

Pebble Games and Linear Equations

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Abstract

We give a new, simplified and detailed account of the correspondence between levels of the Sherali–Adams relaxation of graph isomorphism and levels of pebble-game equivalence with counting (higher-dimensional Weisfeiler–Lehman colour refinement). The correspondence between basic colour refinement and fractional isomorphism, due to Ramana, Scheinerman and Ullman [15], is re-interpreted as the base level of Sherali–Adams and generalised to higher levels in this sense by Atserias and Maneva [1], who prove that the two resulting hierarchies interleave. In carrying this analysis further, we here give (a) a precise characterisation of the level k Sherali–Adams relaxation in terms of a modified counting pebble game; (b) a variant of the Sherali–Adams levels that precisely match the k -pebble counting game; (c) a proof that the interleaving between these two hierarchies is strict. We also investigate the variation based on boolean arithmetic instead of real/rational arithmetic and obtain analogous correspondences and separations for plain k -pebble equivalence (without counting). Our results are driven by considerably simplified accounts of the underlying combinatorics and linear algebra.

Contents

| | | |
|----------|---|-----------|
| 1 | Introduction | 2 |
| 2 | Finite variable logics and pebble games | 4 |
| 3 | Basic combinatorics and linear algebra | 6 |
| 3.1 | Decomposition into irreducible blocks | 7 |
| 3.2 | Eigenvalues and -vectors | 11 |
| 3.3 | Stable partitions | 12 |
| 4 | Fractional isomorphism | 14 |
| 4.1 | C^2 -equivalence and linear equations | 14 |
| 4.2 | L^2 -equivalence and boolean linear equations | 16 |
| 5 | Relaxations in the style of Sherali–Adams | 18 |
| 5.1 | Sherali–Adams of level $k - 1$ | 19 |
| 5.1.1 | From C^k -equivalence to a level $k - 1$ solution | 20 |

| | | |
|-------|--|----|
| 5.1.2 | From a level $k - 1$ solution to $C^{<k}$ -equivalence | 22 |
| 5.2 | The gap | 27 |
| 5.3 | Closing the gap | 31 |
| 5.4 | Boolean arithmetic and L^k -equivalence | 34 |

1 Introduction

We study a surprising connection between equivalence in finite variable logics and a linear programming approach to the graph isomorphism problem. This connection has recently been uncovered by Atserias and Maneva [1], building on earlier work of Ramana, Scheinerman and Ullman [15] that just concerns the 2-variable case.

Finite variable logics play a central role in finite model theory. Most important for this paper are finite variable logics with counting, which have been specifically studied in connection with the question for a logical characterisation of polynomial time and in connection with the graph isomorphism problem (e.g. [5, 7, 8, 11, 12, 14]). Equivalence in finite variable logics can be characterised in terms of simple combinatorial games known as pebble games. Specifically, C^k -equivalence can be characterised by the bijective k -pebble game introduced by Hella [9]. Cai, Fürer and Immerman [5] observed that C^k -equivalence exactly corresponds to indistinguishability by the k -dimensional Weisfeiler-Lehman (WL) algorithm,¹ a combinatorial graph isomorphism algorithm introduced by Babai, who attributed it to work of Weisfeiler and Lehman in the 1970s. The 2-dimensional version of the WL algorithm precisely corresponds to an even simpler isomorphism algorithm known as colour refinement.

The isomorphisms between two graphs can be described by the integral solutions of a system of linear equations. If we have two graphs with adjacency matrices A and B , then each isomorphism from the first to the second corresponds to a permutation matrix X such that $X^tAX = B$, or equivalently

$$AX = XB. \tag{1}$$

If we view the entries of X as variables, this equation corresponds to a system of linear equations. We can add inequalities that force X to be a permutation matrix and obtain a system ISO of linear equations and inequalities whose integral solutions correspond to the isomorphisms between the two graphs. In particular, the system ISO has an integral solution if and only if the two graphs are isomorphic.

What happens if we drop the integrality constraints, that is, we admit arbitrary real solutions of the system ISO? We can ask for doubly stochastic matrices X satisfying equation (1). (A real matrix is *doubly stochastic* if its entries are non-negative and all row sums and column sums are one.) Ramana, Scheinerman and Ullman [15] proved a beautiful result that establishes a connection between linear algebra and logic: the system ISO has a real solution if, and only if, the colour refinement algorithm does not distinguish the two

¹The dimensions of the WL algorithm are counted differently in the literature; what we call “ k -dimensional” here is sometimes called “ $(k - 1)$ -dimensional”.

graphs with adjacency matrices A and B . Recall that the latter is equivalent to the two graphs being \mathcal{C}^2 -equivalent.

To bridge the gap between integer linear programs and their LP-relaxations, researchers in combinatorial optimisation often add additional constraints to the linear programs to bring them closer to their integer counterparts. The Sherali–Adams hierarchy [19] of relaxations gives a systematic way of doing this. For every integer linear program IL in n variables and every positive integer k , there is a *rank- k Sherali–Adams relaxation* $\text{IL}(k)$ of IL, such that $\text{IL}(1)$ is the standard LP-relaxation of IL where all integrality constraints are dropped and $\text{IL}(n)$ is equivalent to IL. There is a considerable body of research studying the strength of the various levels of this and related hierarchies (e.g. [3, 4, 6, 13, 18, 17]).

Quite surprisingly, Atserias and Maneva [1] were able to lift the Ramana–Scheinerman–Ullman result, which we may now restate as an equivalence between $\text{ISO}(1)$ and \mathcal{C}^2 -equivalence, to a close correspondence between the higher levels of the Sherali–Adams hierarchy for ISO and the logics \mathcal{C}^k . They proved for every $k \geq 2$:

1. if $\text{ISO}(k)$ has a (real) solution, then the two graphs are \mathcal{C}^k -equivalent;
2. if the two graphs are \mathcal{C}^k -equivalent, then $\text{ISO}(k - 1)$ has a solution.

Atserias and Maneva used these results to transfer results about the logics \mathcal{C}^k to the world of polyhedral combinatorics and combinatorial optimisation, and conversely, results about the Sherali–Adams hierarchy to logic.

Atserias and Maneva [1] left open the question whether the interleaving between the levels of the Sherali–Adams hierarchy and the finite-variable-logic hierarchy is strict or whether either the correspondence between \mathcal{C}^k -equivalence and $\text{ISO}(k)$ or the correspondence between \mathcal{C}^k -equivalence and $\text{ISO}(k - 1)$ is exact. Note that for $k = 2$ the correspondence between \mathcal{C}^k -equivalence and $\text{ISO}(k - 1)$ is exact by the Ramana–Scheinerman–Ullman theorem. We prove that for all $k \geq 3$ the interleaving is strict. However, we can prove an exact correspondence between $\text{ISO}(k - 1)$ and a variant of the bijective k -pebble game that characterises \mathcal{C}^k -equivalence. This variant, which we call the weak bijective k -pebble game, is actually equivalent to a game called $(k - 1)$ -sliding game by Atserias and Maneva.

Maybe most importantly, we prove that a natural combination of equalities from $\text{ISO}(k)$ and $\text{ISO}(k - 1)$ gives a linear program $\text{ISO}(k - 1/2)$ that characterises \mathcal{C}^k -equivalence exactly.

To obtain these results, we give simple new proofs of the theorems of Ramana, Scheinerman and Ullman and of Atserias and Maneva. Whereas the previous proofs use two non-trivial results from linear algebra, the Perron–Frobenius Theorem (about the eigenvalues of positive matrices) and the Birkhoff–von Neumann Theorem (stating that every doubly stochastic matrix is a convex combination of permutation matrices), our proofs only use elementary linear algebra. This makes them more transparent and less mysterious (at least to us).

In fact, the linear algebra we use is so simple that much of it can be carried out not only over the field of real numbers, but over arbitrary semirings. By

using similar algebraic arguments over the boolean semiring (with disjunction as addition and conjunction as multiplication), we obtain analogous results to those for C^k -equivalence for the ordinary k -variable logic L^k , characterising L^k -equivalence, i.e., k -pebble game equivalence without counting, by systems of ‘linear’ equations over the boolean semiring.

For the ease of presentation, we have decided to present our results only for undirected simple graphs. It is easy to extend all results to relational structures with at most binary relations. Atserias and Maneva did this for their results, and for ours the extension works analogously. An extension to structures with relations of higher arities also seems possible, but is more complicated and comes at the price of loosing some of the elegance of the results.

2 Finite variable logics and pebble games

We assume the reader is familiar with the basics of first-order logic FO. We almost exclusively consider first-order logic over finite graphs, which we view as finite relational structures with one binary relation, and in a few places over other finite relational structures. We assume graphs to be undirected and loop-free. For every positive integer k , we let L^k be the fragment of FO consisting of all formulae that contain at most k distinct variables.

We write $\mathcal{A} \equiv_L^k \mathcal{B}$ to denote that two structures \mathcal{A}, \mathcal{B} are L^k -equivalent, that is, satisfy the same L^k -sentences. L^k -equivalence can be characterised in terms of the k -pebble game, played by two players on a pair \mathcal{A}, \mathcal{B} of structures. A *play* of the game consists of a (possibly infinite) sequence of *rounds*. In each round, player **I** picks up one of his pebbles and places it on an element of one of the structures \mathcal{A}, \mathcal{B} . Player **II** answers by picking up her pebble with the same label and placing it on an element of the other structure.

Note that after each round r there is a subset $p \subseteq \mathcal{A} \times \mathcal{B}$ consisting of the at most k pairs of elements on which the pairs of corresponding pebbles are placed. We call p the *position* after round r . Player **I** wins the play if every position that occurs is a local isomorphism, that is, a local mapping from \mathcal{A} to \mathcal{B} that is injective and preserves membership and non-membership in all relations (adjacency and non-adjacency if \mathcal{A} and \mathcal{B} are graphs).

Theorem 2.1 (Barwise [2], Immerman [10]). $\mathcal{A} \equiv_L^k \mathcal{B}$ if, and only if, player **II** has a winning strategy for the k -pebble game on \mathcal{A}, \mathcal{B} .

We extend L^k -equivalence to structures with distinguished elements. For tuples \mathbf{a} and \mathbf{b} of the same length $\ell \leq k$ we let $\mathcal{A}, \mathbf{a} \equiv_L^k \mathcal{B}, \mathbf{b}$ if \mathcal{A}, \mathbf{a} and \mathcal{B}, \mathbf{b} satisfy the same L^k -formulae $\varphi(\mathbf{x})$ with ℓ free variables \mathbf{x} . The pebble game characterisation extends: $\mathcal{A}, \mathbf{a} \equiv_L^k \mathcal{B}, \mathbf{b}$ if, and only if, player **II** has a winning strategy for the k -pebble game on \mathcal{A}, \mathcal{B} starting with pebbles on \mathbf{a} and the corresponding pebbles on \mathbf{b} . The L^k -type of a tuple \mathbf{a} in a structure \mathcal{A} is the \equiv_L^k -equivalence class of \mathcal{A}, \mathbf{a} . More syntactically, we may also view the L^k -type of \mathbf{a} as the set of all L^k -formulae $\varphi(\mathbf{x})$ satisfied by \mathcal{A}, \mathbf{a} .

Let us turn to the k -variable counting logics. It is convenient to start with the (syntactical) extension C of FO by *counting quantifiers* $\exists^{\geq n}$. The semantics

of these counting quantifiers is the obvious one: $\exists^{\geq n} x \varphi$ means that there are at least n elements x such that φ is satisfied. Of course this can be expressed in FO, but only by a formula that uses at least n variables. For all positive integers k , we let C^k denote the k -variable fragment of C. Whereas C and FO have the same expressive power, C^k is strictly more expressive than L^k .

We write $\mathcal{A} \equiv_C^k \mathcal{B}$ to indicate that structures \mathcal{A} and \mathcal{B} are C^k -equivalent. C^k -equivalence can be characterised in terms of the *bijective k -pebble game*, which, like the k -pebble game, is played by two players by placing k pairs of pebbles on a pair of structures \mathcal{A}, \mathcal{B} . The rounds of the bijective game are as follows. Player **I** picks up one of his pebble, and player **II** picks up her corresponding pebble. Then player **II** chooses a bijection f between \mathcal{A} and \mathcal{B} (if no such bijection exists, that is, if the structures have different cardinalities, player **II** immediately loses). Then player **I** places his pebble on an element a of \mathcal{A} , and player **II** places her pebble on $f(a)$. Again, player **II** wins a play if all positions are local isomorphisms.

Theorem 2.2 (Hella [9]). $\mathcal{A} \equiv_C^k \mathcal{B}$ if, and only if, player **II** has a winning strategy for the bijective k -pebble game on \mathcal{A}, \mathcal{B} .

As L^k -equivalence, we extend C^k -equivalence to structures with distinguished elements, writing $\mathcal{A}, \mathbf{a} \equiv_C^k \mathcal{B}, \mathbf{b}$. Again, the pebble-game characterisation of the equivalence extends. We define C^k -types analogously to L^k -types.

The *colour refinement* algorithm is a simple combinatorial heuristics for testing whether two graphs are isomorphic: Given two graphs \mathcal{A} and \mathcal{B} , which we assume to be disjoint, it computes a colouring of their vertices by the following iterative procedure: Initially, all vertices have the same colour. Then in each round, the colouring is refined by assigning different colours to vertices that have a different number of neighbours of at least one colour assigned in the previous round. Thus after the first round, two vertices have the same colour if, and only if, they have the same degree. After the second round, two vertices have the same colour if, and only if, they have the same degree and for each d the same number of neighbours of degree d . The algorithm stops if no further refinement is achieved; this happens after at most $|\mathcal{A}| + |\mathcal{B}|$ rounds. We call the resulting colouring of $\mathcal{A} \cup \mathcal{B}$ the *stable colouring* of \mathcal{A}, \mathcal{B} . If the stable colouring differs on the two graphs, that is, for some colour c the graphs have a different number of vertices of colour c , then we say that colour refinement *distinguishes* the graphs.

Theorem 2.3 (Immerman and Lander [11]). $\mathcal{A} \equiv_C^2 \mathcal{B}$ if, and only if, colour refinement does not distinguish \mathcal{A} and \mathcal{B} .

The *k -dimensional Weisfeiler-Lehman algorithm* (for short: *k -WL*) is a generalisation of the colour refinement algorithm, which instead of vertices colours k -tuples of vertices. Given two structures \mathcal{A} and \mathcal{B} , which we assume to be disjoint, k -WL iteratively computes a colouring of $\mathcal{A}^k \cup \mathcal{B}^k$. Initially, two tuples $\mathbf{a} = (a_1, \dots, a_k), \mathbf{b} = (b_1, \dots, b_k) \in \mathcal{A}^k \cup \mathcal{B}^k$ get the same colour if the mapping defined by $p(a_i) = b_i$ is a local isomorphism. In each round of the algorithm, the colouring is refined by assigning different colours to tuples that for some

$j \in [k]$ and some colour c have different numbers of j -neighbours of colour c in their respective graphs. Here we call two k -tuples j -neighbours if they differ only in their j th component. The algorithm stops if no further refinement is achieved; this happens after at most $|\mathcal{A}|^k + |\mathcal{B}|^k$ rounds. If after the refinement process the colourings of the two graphs differ, that is, for some colour c the graphs have a different number of k -tuples of colour c , then we say that k -WL distinguishes the graphs.

Theorem 2.4 (Cai, Fürer, and Immerman [5]). $\mathcal{A} \equiv_{\mathbb{C}}^k \mathcal{B}$ if, and only if, k -WL does not distinguish \mathcal{A} and \mathcal{B} .

More significantly, Cai, Fürer, and Immerman [5] proved that for all k there are nonisomorphic graphs $\mathcal{A}_k, \mathcal{B}_k$ of size $O(k)$ such that $\mathcal{A} \equiv_{\mathbb{C}}^k \mathcal{B}$.

Note that the previous two theorems imply that colour refinement and 2-WL distinguish the same graphs.

There are also ‘boolean’ versions of the two algorithms characterising \mathbb{L}^k -equivalence (see [14]).

3 Basic combinatorics and linear algebra

We consider matrices with entries in $\mathbb{B} = \{0, 1\}$, \mathbb{Q} or \mathbb{R} . A matrix $X \in \mathbb{R}^{m,n}$ with m rows and n columns has entry X_{ij} in row $i \in [m] = \{1, \dots, m\}$ and column $j \in [n] = \{1, \dots, n\}$. We write E_n for the n -dimensional unit matrix.

We write $X \geq 0$ to say that (the real or rational) matrix X has only non-negative entries, and $X > 0$ to say that all entries are strictly positive. We also speak of *non-negative* or *strictly positive matrices* in this sense. For a boolean matrix, strict positivity, $X > 0$ means that all entries are 1.

A square $n \times n$ -matrix is *doubly stochastic* if its entries are non-negative and if the sum of entries across every row and column is 1. *Permutation matrices* are doubly stochastic matrices over $\{0, 1\}$, with precisely one 1 in every row and in every column. Permutation matrices are orthogonal, i.e., $PP^t = P^tP = E_n$ for every permutation matrix P . The permutation $p \in S_n$ associated with a permutation matrix $P \in \mathbb{R}^{n,n}$ is such that $Pe_j = e_{p(j)}$, i.e., it describes the permutation of the standard basis vectors that is effected by P . We also say that P represents p . The permutation matrices form a subgroup of the general linear groups. The doubly stochastic matrices do not form a subgroup, but are closed under transpose and product.

It will be useful to have the shorthand notation

$$X_{D_1 D_2} = 0$$

for the assertion that $X_{d_1 d_2} = 0$ for all $d_1 \in D_1$, $d_2 \in D_2$. If p and q are permutations in S_n represented by permutation matrices P and Q , then

$$(P^t X Q)_{D_1 D_2} = 0 \quad \text{iff} \quad X_{p(D_1)q(D_2)} = 0.$$

So, if $X_{D_1 D_2} = 0$ and P and Q are chosen such that $p^{-1}(D_1)$ and $q^{-1}(D_2)$ are final and initial segments of $[n]$, respectively, then $P^t X Q$ has a null block of dimensions $|D_1| \times |D_2|$ in the upper right-hand corner.

3.1 Decomposition into irreducible blocks

Definition 3.1. With $X \in \mathbb{R}^{n,n}$ associate the directed graph

$$G(X) := ([n], \{(i, j) : X_{ij} \neq 0\}).$$

The strongly connected components of $G(X)$ induce a partition of the set $[n] = \{1, \dots, n\}$ of rows/columns of X . X is called *irreducible* if this partition has just the set $[n]$ itself.

Note that X is irreducible iff $P^t X P$ is irreducible for every permutation matrix P .

Observation 3.2. Let $X \in \mathbb{R}^{n,n} \geq 0$ with strictly positive diagonal entries. If X is irreducible, then all powers X^ℓ for $\ell \geq n - 1$ have non-zero entries throughout. Moreover, if X is irreducible, then so is X^ℓ for all $\ell \geq 1$.

Proof. It is easily proved by induction on $\ell \geq 1$ that $(X^\ell)_{ij} \neq 0$ if, and only if there is a directed path of length ℓ from vertex i to vertex j in $G(X)$. For X with positive diagonal entries, $G(X)$ has loops in every vertex, and therefore there is a path of length ℓ from vertex i to vertex j if, and only if, there is path of length M' for every $\ell' \geq \ell$ from i to j . If $G(X)$ is also strongly connected, then any two vertices are linked by a path of length up to $n - 1$. \square

Let us call two matrices $Z, Z' \in \mathbb{R}^{n,n}$ *permutation-similar* or S_n -similar, $Z \sim_{S_n} Z'$, if $Z' = P^t Z P$ for some permutation matrix P , i.e., if one is obtained from the other by a coherent permutation of rows and columns.

Lemma 3.3. Every symmetric $Z \in \mathbb{R}^{n,n} \geq 0$ is permutation-similar to some block diagonal matrix $\text{diag}(Z_1, \dots, Z_s)$ with irreducible blocks $Z_i \in \mathbb{R}^{n_i, n_i}$.

The permutation matrix P corresponding to the row- and column-permutation $p \in S_n$ that puts Z into block diagonal form $P^t Z P = \text{diag}(Z_1, \dots, Z_s)$ with irreducible blocks, is unique up to an outer permutation that re-arranges the block intervals $([k_i + 1, k_i + n_i])_{1 \leq i \leq s}$ where $k_i = \sum_{j < i} n_j$, and a product of inner permutations within each one of these s blocks.

The underlying partition $[n] = \dot{\bigcup}_{1 \leq i \leq s} D_i$ where $D_i := p([k_i + 1, k_i + n_i])$ for $k_i = \sum_{j < i} n_j$, is uniquely determined by Z .²

In the following we refer to the *partition induced by a symmetric matrix Z* .

Proof. Obvious, based on the partition of the vertex set $[n]$ of $G(Z)$ into connected components (note that symmetry of Z is preserved under similarity, and strong connectivity is plain connectivity in $G(Z)$ for symmetric Z). \square

Observation 3.4. In the situation of Lemma 3.3, the partition $[n] = \dot{\bigcup}_i D_i$ induced by the symmetric matrix Z is the partition of $[n]$ into the vertex sets of the connected components of $G(Z)$. Then, for every pair $i \neq j$, $Z_{D_i D_j} = 0$, while all the minors $Z_{D_i D_i}$ are irreducible.³

²Here we regard two partitions as identical if they have the same partition sets, i.e., we ignore their indexing/enumeration.

³Note that this does not depend on the enumeration of the partition set D_i , because irreducibility is invariant under permutation-similarity.

If, moreover, Z has strictly positive diagonal entries, then the partition induced by Z is the same as that induced by Z^ℓ , for any $\ell \geq 1$; for $\ell \geq n-1$, the diagonal blocks $(Z^\ell)_{D_i D_i}$ have non-zero entries throughout: $(Z^\ell)_{D_i D_i} > 0$.

The last assertion says that for a symmetric $n \times n$ matrix Z with non-negative entries and no zeroes on the diagonal, all powers Z^ℓ for $\ell \geq n-1$ are *good symmetric* in the sense of the following definition.

Definition 3.5. Let $Z \geq 0$ be symmetric with strictly positive diagonal. Then Z is called *good symmetric* if w.r.t. the partition $[n] = \dot{\bigcup}_i D_i$ induced by Z , all $Z_{D_i D_i} > 0$.

More generally, a not necessarily symmetric matrix $X \geq 0$ without null rows or columns is *good* if $Z = XX^t$ and $Z' = X^t X$ are good in the above sense.

The importance of this notion lies in the fact that, as observed above, for an arbitrary symmetric $n \times n$ matrix $Z \geq 0$ without zeroes on the diagonal, the partition induced by Z is the same as that induced by the good symmetric matrix $\hat{Z} := Z^{n-1}$; and, as for any good matrix, this partition can simply be read off from \hat{Z} : $i, j \in [n]$ are in the same partition set if, and only if, $\hat{Z}_{ij} \neq 0$.

Definition 3.6. Consider partitions $[n] = \dot{\bigcup}_{i \in I} D_i$ and $[m] = \dot{\bigcup}_{i \in I} D'_i$ of the sets $[n]$ and $[m]$ with the same number of partition sets. We say that these two partitions are *X-related* for some matrix $X \in \mathbb{R}^{n,m}$ if

- (i) $X \geq 0$ has no null rows or columns, and
- (ii) $X_{D_i D'_j} = 0$ for every pair of distinct indices $i, j \in I$.

Note that partitions that are X -related are X^t -related in the opposite direction. More importantly, each one of the X/X^t -related partitions can be recovered from the other one through X according to

$$\begin{aligned} D'_i &= \{d' \in [m] : X_{dd'} > 0 \text{ for some } d \in D_i\}, \\ D_i &= \{d \in [n] : X_{dd'} > 0 \text{ for some } d' \in D'_i\}. \end{aligned}$$

For a more algebraic treatment, we associate with the partition sets D_i of a partition $[n] = \dot{\bigcup}_{i \in I} D_i$ the *characteristic vectors* \mathbf{d}_i with entries 1 and 0 according to whether the corresponding component belongs to D_i :

$$\mathbf{d}_i = \sum_{d \in D_i} \mathbf{e}_d,$$

where \mathbf{e}_d is the d -th standard basis vector. In terms of these characteristic vectors \mathbf{d}_i for $[n] = \dot{\bigcup}_{i \in I} D_i$ and \mathbf{d}'_i for $[m] = \dot{\bigcup}_{i \in I} D'_i$, the X/X^t -relatedness of these partitions means that

$$\begin{aligned} D'_i &= \{d' \in [m] : (X^t \mathbf{d}_i)_{d'} > 0\}, \\ D_i &= \{d \in [n] : (X \mathbf{d}'_i)_d > 0\}. \end{aligned}$$

Lemma 3.7. If two partitions $[n] = \dot{\bigcup}_{i \in I} D_i$ and $[n] = \dot{\bigcup}_{i \in I} D'_i$ of the same set $[n]$ are X -related for some doubly stochastic matrix $X \in \mathbb{R}^{n,n}$, then $|D_i| = |D'_i|$ for all $i \in I$, and for the characteristic vectors \mathbf{d}_i and \mathbf{d}'_i of the partition sets D_i and D'_i even

$$\mathbf{d}_i = X \mathbf{d}'_i \quad \text{and} \quad \mathbf{d}'_i = X^t \mathbf{d}_i.$$

Proof. Observe that for all $d \in [n]$ we have $0 \leq (X\mathbf{d}'_i)_d = \sum_{d' \in D'_i} X_{dd'} \leq 1$. It follows immediately from the definition of X -relatedness that $(X\mathbf{d}'_i)_d = 0$ for all $d \notin D_i$. Therefore,

$$|D_i| \geq \sum_{d \in D_i} (X\mathbf{d}'_i)_d = \sum_{d \in [n]} (X\mathbf{d}'_i)_d = \sum_{d' \in D'_i} \sum_{d \in [n]} X_{dd'} = |D'_i|.$$

Similarly, $0 \leq (X^t\mathbf{d}_i)_{d'} \leq 1$ for $d' \in [n]$, and $|D'_i| \geq \sum_{d' \in D'_i} (X^t\mathbf{d}_i)_{d'} = |D_i|$. Together, we obtain

$$|D_i| = \sum_{d \in D_i} (X\mathbf{d}'_i)_d = |D'_i| = \sum_{d' \in D'_i} (X^t\mathbf{d}_i)_{d'}.$$

As all summands are bounded by 1, this implies $(X\mathbf{d}'_i)_d = 1$ for all $d \in D_i$ and $(X^t\mathbf{d}_i)_{d'} = 1$ for all $d' \in D_i$. \square

Lemma 3.8. *Let $X \geq 0$ be an $m \times n$ matrix without null rows or columns. Then the $m \times m$ matrix $Z := XX^t$ and the $n \times n$ matrix $Z' := X^tX$ are symmetric with positive entries on their diagonals. Moreover, the (unique) partitions of $[m]$ and $[n]$ that are induced by Z and Z' , respectively, are X/X^t -related.⁴*

Proof. It is obvious that Z and Z' are symmetric with positive diagonal entries. Let partitions $[m] = \dot{\bigcup}_{i \in I} D_i$ and $[n] = \dot{\bigcup}_{i \in I'} D'_i$ be obtained from decompositions of Z and Z' into irreducible blocks. We need to show that the non-zero entries in X give rise to a coherent bijection between the index sets I and I' of the two partitions, in the sense that partition sets D_i and D'_j are related if, and only if, some pair of members $d \in D_i$ and $d' \in D'_j$ have a positive entry $X_{dd'}$. Then a re-numbering of one of these partitions will make them X -related in the sense of Definition 3.6. Recall from Observation 3.4 that the D_i are the vertex sets of the connected components of $G(XX^t)$ on $[m]$, while the D'_i are the vertex sets of the connected components of $G(X^tX)$ on $[n]$.

Consider the uniformly directed bipartite graph $G(X)$ on $[m] \dot{\cup} [n]$ with an edge from $i \in [m]$ to $j \in [n]$ if $X_{ij} > 0$. In light of the symmetry of the whole situation w.r.t. X and X^t , it just remains to argue for instance that no $i \in [m]$ can have edges into two distinct sets of the partition $[n] = \dot{\bigcup}_{i \in I'} D'_i$. But any two target nodes of edges from one and the same $i \in [n]$ are in the same connected component of $G(X^tX)$, hence in the same partition set. \square

In the situation of Lemma 3.8, powers of Z induce the same partitions as Z , and the partitions induced by $(Z^\ell X)(Z^\ell X)^t = Z^{2\ell+1}$ are X/X^t -related as well as $Z^\ell X/X^t Z^\ell$ -related, for all $\ell \geq 1$.

For $\ell \geq n/2 - 1$, the matrix $Z^\ell X$ has no null rows or columns: else $Z^\ell X(Z^\ell X)^t = Z^{2\ell+1}$ would have to have a zero entry on the diagonal, contradicting the fact that this symmetric matrix is good symmetric in the sense of Definition 3.5. The same reasoning shows that $Z^\ell X$ is itself good in the sense of Definition 3.5.

⁴As X/X^t -relatedness refers to partitions presented with an indexing of the partition sets, we need to allow a suitable re-indexing for at least one of them, so as to match the other one.

Corollary 3.9. *Let $X \geq 0$ be an $m \times n$ matrix without null rows or columns, $Z = XX^t$, $Z' = X^tX$ the associated symmetric matrices with non-zero entries on the diagonal. Then for $\ell \geq m - 1$, the matrix $\hat{X} := Z^\ell X = X(Z')^\ell$ and its transpose $\hat{X}^t = X^t Z^\ell = (Z')^\ell X^t$ are good and relate the partitions $[m] = \dot{\bigcup}_i D_i$ and $[n] = \dot{\bigcup}_i D'_i$ induced by Z and Z' , respectively.⁴ Moreover,*

- (i) $\hat{X}_{D_i D'_i} > 0$ for all i , and
- (ii) $\hat{X}_{D_i D'_j} = 0$ for all $i \neq j$.

Proof. $Z^\ell X$ is good symmetric by the above reasoning. So $(Z^\ell)_{D_i D_i} > 0$ for all i , while $(Z^\ell)_{D_i D_j} = 0$ for all $j \neq i$. It follows that $(Z^\ell X)_{D_i D'_i} = (Z^\ell)_{D_i D_i} X_{D_i D'_i}$ has only non-zero entries because $X_{D_i D'_i}$ does not have null columns. This proves (i). Assertion (ii) is clear as, for $i \neq j$, $(Z^\ell X)_{D_i D'_j} = (Z^\ell)_{D_i D_j} X_{D_j D'_j} = 0 X_{D_j D'_j} = 0$. \square

Aside: boolean vs. real arithmetic

Looking at matrices with $\{0, 1\}$ -entries, we may not only treat them as matrices over \mathbb{R} as we have done so far, but also over other fields, or as matrices over the boolean semiring $\mathbb{B} = \{0, 1\}$ with the logical operations of \vee for addition and \wedge for multiplication. Though not even forming a ring, boolean arithmetic yields a very natural interpretation in the context where we associate non-negative entries with edges, as we did in passage from X to $G(X)$ (cf. Definition 3.1 and Observation 3.2). The ‘normalisation map’ $\chi: \mathbb{R}_{\geq 0} \rightarrow \{0, 1\}$, $x \mapsto 1$ iff $x > 0$, relates the arithmetic of reals $x, y \geq 0$ to boolean arithmetic in

$$\chi(x + y) = \chi(x) \vee \chi(y) \quad \text{and} \quad \chi(xy) = \chi(x) \wedge \chi(y).$$

This is the ‘logical’ arithmetic that supports, for instance, arguments used in Observation 3.2: for any real $n \times n$ matrix $X \geq 0$, $(XX)_{ij} = \sum_k X_{ik} X_{kj} \neq 0$ iff there is at least one $k \in [n]$ for which $X_{ik} \neq 0$ and $X_{kj} \neq 0$ iff $\bigvee_{k \in [n]} (\chi(X_{ik}) \wedge \chi(X_{kj})) = 1$. It is no surprise, therefore, that several of the considerations apparently presented for real non-negative matrices above, have immediate analogues for boolean arithmetic – in fact, one could argue, that the boolean interpretation is closer to the combinatorial essence. We briefly sum up these analogues with a view to their use in the analysis of \mathbb{L}^k -equivalence, while the real versions are related to \mathbb{C}^k -equivalence. Note also that the boolean analogue of a doubly stochastic matrix with non-negative real entries is a matrix without null rows or columns.

Also note that Definitions 3.1 (irreducibility) and 3.6 (X -relatedness) are applicable to boolean matrices without any changes. Observations 3.2 and 3.4 go through (as just indicated), and so does Lemma 3.3. For Lemma 3.7, one may look at X -related partitions of sets $[m]$ and $[n]$, where not necessarily $n = m$, by any boolean matrix X without null rows or columns and obtains the relationship between the characteristic vectors as stated there, now in terms of boolean arithmetic – but of course we do not get any numerical equalities between the sizes of the partition sets. Lemma 3.8, finally, applies to boolean arithmetic, exactly as stated.

Lemma 3.10. *In the sense of boolean arithmetic for matrices with entries in $\mathbb{B} = \{0, 1\}$:*

- (a) *Any symmetric $Z \in \mathbb{B}^{n,n}$ induces a unique partition of $[n]$ for which the diagonal minors induced by the partition sets are irreducible and the remaining blocks null; $d, d' \in [n]$ are in the same partition set if, and only if, in the sense of boolean arithmetic $(Z^\ell)_{dd'} = 1$ for any/all $\ell \geq n - 1$.*
- (b) *If two partitions (not necessarily of the same set) with the same number of partition sets are related by some boolean matrix $X \in \mathbb{B}^{m,n}$, then the characteristic vectors $(\mathbf{d}_i)_{i \in I}$ and $(\mathbf{d}'_i)_{i \in I}$ of the partitions are related by $\mathbf{d}_i = X\mathbf{d}'_i$ and $\mathbf{d}'_i = X^t\mathbf{d}_i$ in the sense of boolean arithmetic.*
- (c) *For any matrix $X \in \mathbb{B}^{m,n}$ without null rows or columns, the symmetric boolean matrices $Z = XX^t$ and $Z' = X^tX$ have diagonal entries 1 and induce partitions that are X/X^t -related, and agree with the partitions induced by higher powers of Z and Z' or on the basis of $Z^\ell X$ and $X(Z')^\ell$ for any $\ell \in \mathbb{N}$. For $\ell \geq m - 1, n - 1$, the partition blocks in Z and Z' have entries 1 throughout, and $Z^\ell X$ and $X(Z')^\ell$ have entries 1 in all positions relating elements from matching partition sets.*

Observation 3.11. *For a symmetric boolean matrix $Z \in \mathbb{B}^{n,n}$ with $Z_{dd} = 1$ for all $d \in [n]$, the characteristic vectors \mathbf{d}_i of the partition $[n] = \bigcup_{i \in I} D_i$ induced by Z satisfy the following ‘eigenvector’ equation in terms of boolean arithmetic:*

$$Z\mathbf{d}_i = \mathbf{d}_i \quad (\text{boolean}), \quad \text{for all } i \in I.$$

3.2 Eigenvalues and -vectors

Lemma 3.12. *If $Z \in \mathbb{R}^{n,n}$ is doubly stochastic, then it has eigenvalue 1. If Z is doubly stochastic and irreducible with strictly positive diagonal entries, then the eigenspace for eigenvalue 1 has dimension 1 and is spanned by the vector $\mathbf{d} := (1, \dots, 1)^t$.*

Proof. Clearly $Z\mathbf{d} = \mathbf{d}$ for any stochastic matrix Z .

If Z is moreover irreducible with positive diagonal entries, then by Observation 3.2, $Z^* := Z^{n-1}$ has strictly positive entries and, being doubly stochastic, therefore entries strictly between 0 and 1.

If \mathbf{v} is an eigenvector for eigenvalue 1 of Z , then also of Z^* . If $\mathbf{v} = (v_1, \dots, v_n)$, this is equivalent to

$$v_i = \sum_j Z_{ij}^* v_j \quad \text{for all } i \in [n].$$

Looking at an index i for which $v_j \leq v_i$ for all j , we see that the maximal v_i is a convex combination of the v_j to which every v_j contributes. This implies that all $v_j = v_i$, so that \mathbf{v} is a scalar multiple of \mathbf{d} as claimed. \square

Corollary 3.13. (a) *Let $Z \in \mathbb{R}^{n,n}$ be doubly stochastic with positive diagonal, and $[n] = \bigcup_i D_i$ a partition with $Z_{D_i D_j} = 0$ for $i \neq j$ and such that the minors $Z_{D_i D_i}$ are irreducible for all i . Then the eigenspace for eigenvalue 1 of Z is the direct sum of the 1-dimensional subspaces spanned by the characteristic vectors \mathbf{d}_i of the partition sets D_i .*

- (b) If $Z = X^t X \in \mathbb{R}^{n,n}$ for some doubly stochastic matrix X , then the eigenspace for eigenvalue 1 is the direct sum of the spans of the characteristic vectors \mathbf{d}_i from the unique partition $[n] = \dot{\bigcup}_i D_i$ of $[n]$ induced by Z according to Lemma 3.3.

Proof. Towards (a), it is clear that $Z\mathbf{d}_i = \mathbf{d}_i$, so that each \mathbf{d}_i is an eigenvector with eigenvalue 1. Let $V_i := \text{span}(\mathbf{e}_d : d \in D_i)$; then $\mathbb{R}^n = \bigoplus_i V_i$ is a direct sum decomposition, and $Z_{D_j D_i} = 0$ for $j \neq i$ implies that Z maps V_i to itself. Therefore any eigenvector \mathbf{v} with eigenvalue 1 decomposes as $\mathbf{v} = \sum_i \mathbf{v}_i$, where $\mathbf{v}_i \in V_i$, in such manner that $Z\mathbf{v}_i = \mathbf{v}_i$. Since the restriction of Z to V_i is irreducible with positive diagonal, $\mathbf{v}_i \in \text{span}(\mathbf{d}_i)$ by Lemma 3.12, as claimed.

Statement (b) is a direct consequence, since Z is symmetric with positive diagonal. \square

3.3 Stable partitions

Definition 3.14. Let $A \in \mathbb{R}^{n,n}$, $[n] = \dot{\bigcup}_{i \in I} D_i$ be a partition. We call this partition a *stable partition* for A if there are numbers $(s_{ij})_{i,j \in I}$ and $(t_{ij})_{i,j \in I}$ such that for all $i, j \in I$:

$$d \in D_i \quad \Rightarrow \quad \sum_{d' \in D_j} A_{dd'} = s_{ij} \quad \text{and} \quad \sum_{d' \in D_j} A_{d'd} = t_{ij}.$$

If there are s_{ij} such that $\sum_{d' \in D_j} A_{dd'} = s_{ij}$ for all $d \in D_i$, we call the partition *row-stable*; similarly, for t_{ij} such that $\sum_{d' \in D_j} A_{d'd} = t_{ij}$ for all $d \in D_i$, *column-stable*.

For symmetric A , column- and row-stability are equivalent (with $t_{ij} = s_{ij}$).

Note that the row and column sums in the definition are the D_i -components of $A\mathbf{d}_j$ and of $\mathbf{d}_j^t A = (A^t \mathbf{d}_j)^t$, respectively. So, for instance, row stability precisely says that

$$A\mathbf{d}_j = \sum_i s_{ij} \mathbf{d}_i \in \bigoplus_i \text{span}(\mathbf{d}_i).$$

Lemma 3.15. Let $A \in \mathbb{R}^{n,n}$ commute with some symmetric matrix of the form $Z = XX^t \in \mathbb{R}^{n,n}$ for some doubly stochastic $X \in \mathbb{R}^{n,n}$. Then the partition $[n] = \dot{\bigcup}_i D_i$ of $[n]$ induced by Z according to Lemma 3.3 is stable for A .

Proof. We use the characteristic vectors \mathbf{d}_i of the partition sets. By Corollary 3.13, the eigenspace for eigenvalue 1 of Z is the direct sum of the spans of the vectors \mathbf{d}_i .

Now $Z A \mathbf{d}_i = A Z \mathbf{d}_i = A \mathbf{d}_i$ shows that $A \mathbf{d}_i$ is an eigenvector of Z with eigenvalue 1, whence

$$A \mathbf{d}_i \in \bigoplus_i \text{span}(\mathbf{d}_i).$$

It follows that the partition $[n] = \dot{\bigcup}_i D_i$ is row-stable.

Note again that $(A\mathbf{d}_j)_d = \sum_{d' \in D_j} A_{dd'}$ and $A\mathbf{d}_j \in \bigoplus_i \text{span}(\mathbf{d}_i)$ precisely means that this value $(A\mathbf{d}_j)_d$ only depends on the partition set D_i to which d belongs. I.e., $\sum_{d' \in D_j} A_{dd'} = s_{ij}$ for all $d \in D_i$.

As $Z = XX^t = Z^t$, A^t commutes with Z if A does: $A^t Z = A^t Z^t = (ZA)^t = (AZ)^t = Z^t A^t = ZA^t$. The above reasoning therefore shows that the partition into the D_i is row-stable for A^t as well, hence column stable for A . Hence it is stable for A . \square

NB: symmetry of A is not required here. It is essential for deriving commutation of A (and A^t) with $Z = XX^t$ from an equation of the form $AX = XB$, as we shall see below. But first a corollary from the argument just given.

Corollary 3.16. *Let A commute with $Z = XX^t$ and B commute with $Z' = X^t X$, where X is doubly stochastic (cf. Lemma 3.15). Then the partitions induced by Z and Z' , which are X -related by Lemma 3.8, are stable for A and B , respectively.*

Aside: boolean arithmetic

We give a separate elementary proof of the analogue of Lemma 3.15 for boolean arithmetic. Here the definition of a *boolean* stable partition is this natural analogue of Definition 3.14.

Definition 3.17. A partition $[n] = \dot{\bigcup}_{i \in I} D_i$ is *boolean stable* for $A \in \mathbb{B}^{n,n}$ if, in the sense of boolean arithmetic, $\sum_{d' \in D_j} A_{dd'}$ and $\sum_{d' \in D_j} A_{d'd}$ only depend on the partition set i for which $d \in D_i$.

Note that boolean stability implies that, for the characteristic vectors \mathbf{d}_i of the partition, $(A\mathbf{d}_j)_d = \sum_{d' \in D_j} A_{dd'}$ is the same for all $d \in D_i$, so that also here $A\mathbf{d}_j$ is a boolean linear combination of the characteristic vectors \mathbf{d}_i .

Lemma 3.18. *Let $A \in \mathbb{B}^{n,n}$ commute, in the sense of boolean arithmetic, with some symmetric matrix of the form $Z = XX^t \in \mathbb{B}^{n,n}$ with entries $Z_{dd} = 1$ for all $d \in [n]$. Then the partition $[n] = \dot{\bigcup}_i D_i$ induced by Z according to Lemma 3.10 is boolean stable for A .*

Proof. Recall from Observation 3.11 that the characteristic vectors \mathbf{d}_i of the induced partition behave like eigenvector with eigenvalue 1 for boolean arithmetic: $Z\mathbf{d}_i = \mathbf{d}_i$. Moreover, we may assume that $Z_{dd'} = 1$ iff d and d' are in the same partition set (after passage to Z^{n-1} if necessary). Let us write $\llbracket \ell \in D_j \rrbracket$ for the boolean truth value of the assertion $\ell \in D_j$. Then, for $d \in D_i$,

$$\begin{aligned} \sum_{d' \in D_j} A_{dd'} &= (A\mathbf{d}_j)_d = (AZ\mathbf{d}_j)_d \\ &= (ZA\mathbf{d}_j)_d = \sum_{k, \ell} Z_{dk} A_{k\ell} \llbracket \ell \in D_j \rrbracket = \sum_{k \in D_i, \ell \in D_j} A_{k\ell} \end{aligned}$$

does indeed not depend on $d \in D_i$, whence the partition is boolean row-stable. Column-stability again follows from similar considerations based on commutation of $Z = Z^t$ with A^t . \square

4 Fractional isomorphism

4.1 \mathbf{C}^2 -equivalence and linear equations

The *adjacency matrix* of graph \mathcal{A} is the square matrix A with rows and columns indexed by vertices of \mathcal{A} and entries $A_{aa'} = 1$ if aa' is an edge of \mathcal{A} and $A_{aa'} = 0$ otherwise. By our assumption that graphs are undirected and simple, A is a symmetric square matrix with null diagonal. It will be convenient to assume that our graphs always have an initial segment $[n]$ of the positive integers as their vertex set. Then the adjacency matrices are in $\mathbb{B}^{n,n} \subseteq \mathbb{R}^{n,n}$. Throughout this subsection, we assume that \mathcal{A} and \mathcal{B} are graphs with vertex set $[n]$ and with adjacency matrices A, B , respectively. It will be notationally suggestive, to denote typical indices of matrices $a, a', \dots \in [n]$ when they are to be interpreted as vertices of \mathcal{A} , and $b, b', \dots \in [n]$ when they are to be interpreted as vertices of \mathcal{B} .

Recall (from the discussion in the introduction) that two graphs \mathcal{A}, \mathcal{B} are isomorphic if, and only if, there is a permutation matrix X such that $AX = XB$. We can rewrite this as the following integer linear program in the variables X_{ab} for $a, b \in [n]$.

ISO

$$\begin{aligned} \sum_{b' \in [n]} X_{ab'} &= \sum_{a' \in [n]} X_{a'b} = 1, \\ \sum_{a' \in [n]} A_{aa'} X_{a'b} &= \sum_{b' \in [n]} X_{ab'} B_{b'b}, \\ X_{ab} &\geq 0 \end{aligned} \quad \text{for all } a, b \in [n].$$

Then \mathcal{A} and \mathcal{B} are isomorphic if, and only if, ISO has an integer solution.

Definition 4.1. *Two graphs \mathcal{A}, \mathcal{B} are fractionally isomorphic, $\mathcal{A} \approx \mathcal{B}$, if, and only if, the system ISO has a real solution.*

Observe that graphs are fractionally isomorphic if, and only if, there is a doubly stochastic matrix X such that $AX = XA$.

Note that fractionally isomorphic graphs necessarily have the same number of vertices (this will be different for the boolean analogue, which cannot count).

The established theorem on fractional isomorphism, by Ramana, Scheinerman and Ullman from [15, 16], relates fractional isomorphism to the colour refinement algorithm (‘iterated degree sequences’ in [16]) introduced in Section 2 and stable partitions (‘equitable partitions’ in [16]).

A *stable partition* of the vertex set of an undirected graph is a stable partition $[n] = \bigcup_{i \in I} D_i$ for its adjacency matrix in the sense of Definition 3.14. Reading that definition for the (symmetric) adjacency matrix A of a graph on $[n]$, and thinking of the partition sets D_i as vertex colours, stability means that the colour of any vertex determines the number of its neighbours in every one of the colours. This is stability in the sense of colour refinement; it means that the colour refinement algorithm produces the coarsest stable partition.

The characteristic parameters for a stable partition $[n] = \dot{\bigcup}_{i \in I} D_i$ for A are the numbers $s_{ij} = s_{ij}^A$ such that $s_{ij} = \sum_{d' \in D_j} A_{dd'}$ for all $d \in D_i$. (As A is symmetric, the parameters t_{ij} of Definition 3.14 are equal to the s_{ij} .) We call two stable partitions $\dot{\bigcup}_{i \in I} D_i$ for a matrix A and $\dot{\bigcup}_{i \in J} D'_i$ for a matrix B *equivalent* if $I = J$ and $|D_i| = |D'_i|$ for all $i \in I$ and $s_{ij}^A = s_{ij}^B$ and for all $i, j \in I$.

Lemma 4.2. *\mathcal{A} and \mathcal{B} are \mathcal{C}^2 -equivalent if, and only if, there are equivalent stable partitions $\dot{\bigcup}_{i \in I} D_i$ for A and $\dot{\bigcup}_{i \in I} D'_i$ for B .*

Proof. The forward direction follows from Theorem 2.3, because the colour refinement algorithm computes equivalent stable partitions of \mathcal{A} and \mathcal{B} .

To establish the converse implication, we use the bijective 2-pebble game, which characterises \mathcal{C}^2 -equivalence by Theorem 2.2. Suppose we have equivalent stable partitions $\dot{\bigcup}_{i \in I} D_i$ of A and $\dot{\bigcup}_{i \in J} D'_i$ of B . Then it is a winning strategy for player **II** to maintain the following invariant for every position p of the game: p is a local isomorphism (that is, if $\text{dom}(p) = \{a, a'\}$ then $a = a'$ if, and only if, $p(a) = p(a')$, and a and a' are adjacent in \mathcal{A} if, and only if, $p(a)$ and $p(a')$ are adjacent in \mathcal{B}), and if $a \in \text{dom}(p) \cap D_i$ then $p(a) \in D'_i$. It follows easily from the definition of stable partitions that player **II** can indeed maintain this invariant. \square

Theorem 4.3 (Ramana–Scheinerman–Ullman). *Two graphs are \mathcal{C}^2 -equivalent if, and only if, they are fractionally isomorphic.*

Proof. In view of Lemma 4.2, it suffices to prove that \mathcal{A} and \mathcal{B} have equivalent stable partitions if, and only if, they are fractionally isomorphic.

For the forward direction, suppose that we have equivalent stable partitions $\dot{\bigcup}_{i \in I} D_i$ for A and $\dot{\bigcup}_{i \in J} D'_i$ for B . For all $a \in D_i, b \in D'_j$ we let

$$X_{ab} := \delta(i, j) / n_i,$$

where $n_i := |D_i| = |D'_i|$. (Here and elsewhere we use Kronecker's δ function defined by $\delta(i, j) = 1$ if $i = j$ and $\delta(i, j) = 0$ otherwise.) An easy calculation shows that this defines a doubly stochastic matrix X with $AX = XB$, that is, a solution for ISO.

For the converse direction, suppose that X is a doubly stochastic matrix such that $AX = XB$. Since A and B are symmetric, also $X^t A = B X^t$, and

$$A X X^t = X B X^t = X X^t A \quad \text{and} \quad B X^t X = X^t A X = X^t X B,$$

show that A commutes with $Z := X X^t$ and B with $Z' := X^t X$.

From Lemma 3.15 and Corollary 3.16, the partitions $[n] = \dot{\bigcup}_{i \in I} D_i$ and $[n] = \dot{\bigcup}_{i \in I} D'_i$ that are induced by the symmetric matrices Z and Z' are X -related and stable for A and for B , respectively. We need to show that $|D_i| = |D'_i|$ and that the partitions also agree w.r.t. the parameters s_{ij} .

By Lemma 3.7 we have $|D_i| = |D'_i|$ and

$$\mathbf{d}_i = X \mathbf{d}'_i \quad \text{and} \quad \mathbf{d}'_i = X^t \mathbf{d}_i, \tag{2}$$

where \mathbf{d}_i and \mathbf{d}'_i for $i \in I$ are the characteristic vectors of the two partitions. Thus for all $i, j \in I$,

$$(\mathbf{d}'_i)^t B \mathbf{d}'_j = (X^t \mathbf{d}_i)^t B X^t \mathbf{d}_j = \mathbf{d}_i^t X B X^t \mathbf{d}_j = \mathbf{d}_i^t A X X^t \mathbf{d}_j = \mathbf{d}_i^t A Z \mathbf{d}_j = \mathbf{d}_i^t A \mathbf{d}_j,$$

where the last equality follows from the fact that \mathbf{d}_j is an eigenvector of Z with eigenvalue 1 by Corollary 3.13.

Note that $\mathbf{d}_i^t A \mathbf{d}_j$ is the number of edges of \mathcal{A} from D_i to D_j . By stability of the partition, we have $s_{ij}^A = \mathbf{d}_i^t A \mathbf{d}_j / |D_i|$ and similarly $s_{ij}^B = (\mathbf{d}'_i)^t B \mathbf{d}'_j / |D'_i|$, so that $s_{ij}^A = s_{ij}^B$. \square

4.2 L^2 -equivalence and boolean linear equations

W.r.t. an adjacency matrix $A \in \mathbb{B}^{n,n}$, a boolean stable partition $[n] = \dot{\bigcup}_{i \in I} D_i$ has as parameters just the boolean values

$$\iota_{ij}^A = \begin{cases} 0 & \text{if } A_{D_i D_j} = 0, \\ 1 & \text{else.} \end{cases}$$

Boolean (row-)stability of the partition for A implies that $\iota_{ij}^A = 1$ if, and only if, for each individual $d \in D_i$ there is at least one $d' \in D_j$ such that $A_{dd'} = 1$, and similarly for column stability.

To capture the situation of 2-pebble game equivalence, though, we now need to work with similar partitions that are stable both w.r.t. A and w.r.t. to the adjacency matrix A^c of the complement of the graph with adjacency matrix A . Here the complement of a graph \mathcal{A} is the graph \mathcal{A}^c with the same vertex set as \mathcal{A} obtained by replacing edges by non-edges and vice versa. Hence $A_{aa'}^c = 1$ if $A_{aa'} = 0$ and $a \neq a'$, and $A_{aa'}^c = 0$ otherwise. While a partition in the sense of real arithmetic is stable for A if, and only if, it is stable for A^c , this is no longer the case for boolean arithmetic. Let us call a partition that is boolean stable for both A and A^c , *boolean bi-stable* for A .

Then the following captures the situation of two graphs that are 2-pebble game equivalent. We note that 2-pebble equivalence is a very rough notion of equivalence, if we look at just simple undirected graphs – but the concepts explored here do have natural extensions to coloured, directed graphs, and form the basis for the analysis of k -pebble equivalence, which is non-trivial even for simple undirected graphs.

L^2 -equivalence of two graphs does not imply that the graphs have the same size. In the following, we always assume that \mathcal{A}, \mathcal{B} are graphs with vertex sets $[m], [n]$ respectively and that $A \in \mathbb{B}^{m,m}$ and $b \in \mathbb{B}^{n,n}$ are their adjacency matrices. We call two bi-stable partitions $[m] = \dot{\bigcup}_{i \in I} D_i$ for A (and A^c) and $[n] = \dot{\bigcup}_{i \in J} D'_i$ for B (and B^c) *b-equivalent* if $I = J$ and $\iota_{ij}^A = \iota_{ij}^B$ and $\iota_{ij}^{A^c} = \iota_{ij}^{B^c}$ and for all $i, j \in I$. Note that b-equivalence does not imply that $|D_i| = |D'_i|$.

Lemma 4.4. *\mathcal{A} and \mathcal{B} are L^2 -equivalent if, and only if, there are b-equivalent bi-stable partitions $[m] = \dot{\bigcup}_{i \in I} D_i$ for A and $[n] = \dot{\bigcup}_{i \in J} D'_i$ for B .*

Proof. The proof is analogous to the proof of Lemma 4.4. For the backward direction, we need bistability to guarantee that player **II** can maintain position p that preserve adjacency, non-adjacency, and (in)equality. Stability alone would only enable her to maintain adjacency and equality. \square

Definition 4.5. \mathcal{A} and \mathcal{B} are *boolean isomorphic*, $\mathcal{A} \approx_{\text{bool}} \mathcal{B}$, if there is some boolean matrix X without null rows or columns such that $AX = XB$ and $A^c X = XB^c$.

Theorem 4.6. *Two graphs are L^2 -equivalent if, and only if, they are boolean isomorphic.*

Proof. For the forward direction, suppose that $A \equiv_L^2 B$, and let $[m] = \dot{\bigcup}_{1 \leq i \leq s} D_i$ and $[n] = \dot{\bigcup}_{1 \leq i \leq s} D'_i$ be the similar boolean bi-stable partitions. For all $a \in D_i, b \in D'_j$ we let $X_{ab} := \delta(i, j)$. This defines a boolean matrix $X \in \mathbb{B}^{m,n}$ without null rows or columns. One checks that $AX = XB$, in boolean arithmetic: for $a \in D_i$ and $b \in D'_j$, and for the characteristic vectors \mathbf{d}_i and \mathbf{d}'_j for the partitions,

$$\begin{aligned} (AX)_{ab} &= \sum_k A_{ak} X_{kb} = (A\mathbf{d}_j)_a = \iota_{ij}^A \\ &= \iota_{ij}^B = (B\mathbf{d}'_i)_b = ((\mathbf{d}'_i)^t B^t)_b = \sum_k X_{ak} B_{kb} = (XB)_{ab}. \end{aligned}$$

The argument for $A^c X = XB^c$ is completely analogous.

For the converse, suppose that $A \approx_{\text{bool}} B$, and let X be a boolean matrix without null rows or columns such that $AX = XB$ and $A^c X = XB^c$. Since A and B are symmetric, also $X^t A = BX^t$ $X^t A^c = B^c X^t$, and

$$AXX^t = XBX^t = XX^t A \quad \text{and} \quad BX^t X = X^t AX = X^t XB,$$

and the analogue for the complements, show that both A and A^c commute with $Z := XX^t$ and both B and B^c commute with $Z' := X^t X$. Moreover, the matrices Z and Z' have entries 1 on the diagonal.

From Lemma 3.18 and the straightforward analogue of Corollary 3.16, the partitions $[m] = \dot{\bigcup}_{i \in I} D_i$ and $[n] = \dot{\bigcup}_{i \in I} D'_i$ induced by the symmetric matrices Z and Z' are X -related and boolean bi-stable for A and for B , respectively. We need to show that these partitions also agree w.r.t. the characteristic ι_{ij} . By Lemma 3.10, the characteristic vectors \mathbf{d}'_i and \mathbf{d}_i of the partitions are related by $\mathbf{d}_i = X\mathbf{d}'_i$ and $\mathbf{d}'_i = X^t \mathbf{d}_i$ in the sense of boolean arithmetic.

Since $AX = XB$ and as the \mathbf{d}_j are boolean eigenvectors of $Z = XX^t$ with eigenvalue 1 by Observation 3.11,

$$\begin{aligned} \iota_{ij}^B &= (\mathbf{d}'_i)^t B \mathbf{d}'_j = (X^t \mathbf{d}_i)^t B X^t \mathbf{d}_j = \mathbf{d}_i^t X B X^t \mathbf{d}_j \\ &= \mathbf{d}_i^t A X X^t \mathbf{d}_j = \mathbf{d}_i^t A Z \mathbf{d}_j = \mathbf{d}_i^t A \mathbf{d}_j = \iota_{ij}^A. \end{aligned}$$

The argument for $\iota_{ij}^{B^c} = \iota_{ij}^{A^c}$ is strictly analogous. \square

5 Relaxations in the style of Sherali–Adams

In this section we refine the connection between the Sherali–Adams hierarchy of LP relaxation of the integer linear program ISO to equivalence in the finite variable counting logics or the higher-dimensional Lehman–Weisfeiler equivalence.

NB: our parameter $k \geq 2$ is the number of pebbles, or the variables available in the k -variable logics \mathcal{C}^k or \mathcal{L}^k .

As before, \mathcal{A} and \mathcal{B} are graphs with vertex sets $[m]$ and $[n]$, respectively, and A and B are their adjacency matrices. We denote typical elements and tuples of elements from \mathcal{A} and \mathcal{B} as $\mathbf{a} = (a_1, \dots, a_r)$ or $\mathbf{b} = (b_1, \dots, b_r)$, for $0 \leq r \leq k$; correspondingly, we typically denote entries of the adjacency matrices as, e.g., $A_{aa'}$. This device will help in an intuitive consistency check also in matrix compositions like AX with entries $(AX)_{ab}$ if A is an $m \times m$ matrix over $[m]$ and X , as an $m \times n$ matrix, relates $[m]$ and $[n]$ through entries X_{ab} : $(AX)_{ab} = \sum_{a'} A_{aa'} X_{a'b}$ (which rightly suggests paths of length two in a suitable composition of graphs \mathcal{A} and $G(X)$).

Types. Let $\text{etp}(\mathbf{a})$ denote the equality type of tuple \mathbf{a} in \mathcal{A} , $\text{atp}(\mathbf{a})$ its quantifier-free type, and $\text{tp}(\mathbf{a})$ its complete type in the logic \mathcal{C}^k , that is, the set of all \mathcal{C}^k -formulae $\varphi(\mathbf{x})$ such that \mathcal{A} satisfies $\varphi(\mathbf{a})$. Note that $\mathbf{a} \mapsto \mathbf{b}$ constitutes a local bijection if, and only if, $\text{etp}(\mathbf{a}) = \text{etp}(\mathbf{b})$, and a local isomorphism if, and only if $\text{atp}(\mathbf{a}) = \text{atp}(\mathbf{b})$.

Types with parameters are denoted as in $\text{tp}_{\mathbf{a}}(a)$ for the type of a w.r.t. to the fixed parameter tuple \mathbf{a} ; we may treat types as if they were formulae, with free variables for the main argument (as opposed to the parameter tuple), as in $(\text{tp}_{\mathbf{a}}(a))$ viewed as a formula with parameters for \mathbf{a} and a free variable x assuming the role of a . By logics with restrictions on the number of variables, however, these parameters are accessible as assignments to variables; they thus count towards the variables in formulae, and are not treated as constants. The distinction between plain types and types with parameters, therefore, is one of semantic intention rather than syntactic. It is often suggestive when it comes to counting realisations. E.g., we let

$$\#_{\mathbf{x}}^{\mathcal{A}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a}))$$

denote the number of tuples \mathbf{a}' in \mathcal{A} that realise the type of \mathbf{a} , i.e., those \mathbf{a}' for which $\mathcal{A}, \mathbf{a}' \equiv_{\mathcal{C}^k}^{\mathcal{A}} \mathcal{A}, \mathbf{a}$. If the structure in which realisations are counted is obvious or does not matter because of \mathcal{C}^k -equivalence, we drop the superscript and write e.g. just $\#_{\mathbf{x}}$ instead of $\#_{\mathbf{x}}^{\mathcal{A}}$ or $\#_{\mathbf{x}}^{\mathcal{B}}$.

The number of realisations of the 1-type of a over parameters \mathbf{a} (in \mathcal{A}) is denoted by

$$\#_x(\text{tp}_{\mathbf{a}}(x) = \text{tp}_{\mathbf{a}}(a)) \quad (= \#_x(\text{tp}(\mathbf{a}x) = \text{tp}(\mathbf{a}a))).$$

Regarding the counting of realisations we note that generally

$$\#_{\mathbf{x}x}(\text{tp}(\mathbf{x}x) = \text{tp}(\mathbf{a}a)) \quad = \quad \#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})) \cdot \#_x(\text{tp}_{\mathbf{a}}(x) = \text{tp}_{\mathbf{a}}(a)). \quad (3)$$

The equations. In the following we use variables X_p indexed by subsets $p \subseteq [m] \times [n]$ of size up to $k-1$; we may think of such p as being specified by two tuples \mathbf{a} and \mathbf{b} of length $|p|$ that enumerate the first and second components of the pairs in p in any coherent order. In this sense we write $p = \mathbf{ab}$. As remarked before, p is a local bijection between \mathcal{A} and \mathcal{B} iff $\text{etp}(\mathbf{a}) = \text{etp}(\mathbf{b})$, and a local isomorphism iff $\text{atp}(\mathbf{a}) = \text{atp}(\mathbf{b})$ (and neither of these conditions depends on the chosen enumeration of tuples in p , which gives rise to the order of components in both \mathbf{a} and \mathbf{b}).

The augmentation of $p \subseteq [m] \times [n]$ by some pair $ab \in [m] \times [n]$ is simply denoted $p \hat{\sim} ab$. It is crucial that the notation $p \hat{\sim} ab$ does not refer to a *tuple* of pairs but to a *set* of pairs, in which the pair (a, b) is not distinguished.

For further reference we isolate and name equation types as follows. For given $n, m \geq 1$ and matrices $A \in \mathbb{B}^{n,n}$ and $B \in \mathbb{B}^{m,m}$:

$$\begin{array}{ll}
X_\emptyset = 1 & \text{CONT}(0) \\
\left. \begin{array}{l} X_p = \sum_{b'} X_{p \hat{\sim} ab'} = \sum_{a'} X_{p \hat{\sim} a'b} \\ \text{for } |p| = \ell - 1, a \in [m], b \in [n] \end{array} \right\} & \text{CONT}(\ell) \\
\left. \begin{array}{l} \sum_{a'} A_{aa'} X_{p \hat{\sim} a'b} = \sum_{b'} X_{p \hat{\sim} ab'} B_{b'b} \\ \text{for } |p| = \ell - 1, a \in [m], b \in [n] \end{array} \right\} & \text{COMP}(\ell)
\end{array}$$

Here *level* ℓ refers to ℓ as the size of the pairings \mathbf{ab} in the typical variables $X_{\mathbf{ab}}$ involved; note that the size of p mentioned in $X_{p \hat{\sim} ab}$ therefore remains one below this ℓ . In the generic formats for $\text{CONT}(\ell)$ and $\text{COMP}(\ell)$ above, we assume $\ell \geq 1$. Note that the combination of $\text{CONT}(\ell)$ and $\text{COMP}(\ell)$ for $\ell = 1$ precisely corresponds to the equations for fractional isomorphism.

If we think of the matrix entries $(X_{\mathbf{ab} \hat{\sim} ab})_{a \in [n], b \in [m]}$ as specifying extensions of $\mathbf{a} \mapsto \mathbf{b}$ in form of a distribution on possible pairings $a \mapsto b$, then equations $\text{CONT}(\ell)$ may be seen as *continuity conditions*, while equations $\text{COMP}(\ell)$ specify *compatibility conditions* with the edge relations encoded in A and B . Variants of the compatibility conditions can be expressed for matrices other than the adjacency matrices A and B that we primarily think of. We saw one such variation in the discussion on boolean isomorphisms above, where $\text{COMP}(1)$ was postulated for both A, B and A^c, B^c . Further variants will play a role in Section 5.4.

5.1 Sherali–Adams of level $k-1$

For $k \geq 2$, the *level- $(k-1)$ Sherali–Adams relaxation* of the integer linear program ISO consists of the collection of the equations $\text{CONT}(\ell)$ and $\text{COMP}(\ell)$ for $\ell < k$:

| | |
|---|--|
| $\text{ISO}(k-1)$ <div style="display: flex; justify-content: space-between; align-items: center; margin-top: 10px;"> <div style="flex: 1;"> $\left. \begin{aligned} X_\emptyset &= 1 \quad \text{and} \\ X_p &= \sum_{b'} X_{p \wedge ab'} = \sum_{a'} X_{p \wedge a'b} \\ \text{for } p < k-1, a \in [m], b \in [n] \end{aligned} \right\}$ </div> <div style="flex: 1; text-align: center;"> $\text{CONT}(\ell) \text{ for } \ell < k$ </div> </div> <div style="display: flex; justify-content: space-between; align-items: center; margin-top: 10px;"> <div style="flex: 1;"> $\left. \begin{aligned} \sum_{a'} A_{aa'} X_{p \wedge a'b} &= \sum_{b'} X_{p \wedge ab'} B_{b'b} \\ \text{for } p < k-1, a \in [m], b \in [n] \end{aligned} \right\}$ </div> <div style="flex: 1; text-align: center;"> $\text{COMP}(\ell) \text{ for } \ell < k$ </div> </div> <div style="margin-top: 10px;"> $X_p \geq 0 \text{ for } p \leq k-1$ </div> | |
|---|--|

5.1.1 From \mathbf{C}^k -equivalence to a level $k-1$ solution

Assume that $\mathcal{A} \equiv_{\mathbf{C}}^k \mathcal{B}$. This implies that \mathcal{A} and \mathcal{B} realise exactly the same types of r -tuples for $r \leq k$ and with the same number of realisations:

$$\#_{\mathbf{x}}^{\mathcal{A}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})) = \#_{\mathbf{x}}^{\mathcal{B}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})) \quad (4)$$

and similarly for all types $\text{tp}(\mathbf{b})$ of r -tuples in \mathcal{B} for $r \leq k$. In particular $m = |\mathcal{A}| = |\mathcal{B}| = n$ so that both structures have domain $[n]$.

If $\text{tp}(\mathbf{a}) = \text{tp}(\mathbf{b})$, where \mathbf{a} and \mathbf{b} are r -tuples for $r \leq k-1$, then, for any $a \in [n]$, there are $\hat{b} \in [n]$ such that $\text{tp}(\mathbf{b}\hat{b}) = \text{tp}(\mathbf{a}a)$; and for any such choice of \hat{b} we find (cf. equation (3)):

$$\begin{aligned} \#_x^{\mathcal{A}}(\text{tp}_{\mathbf{a}}(x) = \text{tp}_{\mathbf{a}}(a)) &= \#_{\mathbf{x}x}^{\mathcal{A}}(\text{tp}(\mathbf{x}x) = \text{tp}(\mathbf{a}a)) / \#_{\mathbf{x}}^{\mathcal{A}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})) \\ &= \#_{\mathbf{x}x}^{\mathcal{B}}(\text{tp}(\mathbf{x}x) = \text{tp}(\mathbf{a}a)) / \#_{\mathbf{x}}^{\mathcal{B}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})) \\ &= \#_{\mathbf{x}x}^{\mathcal{B}}(\text{tp}(\mathbf{x}x) = \text{tp}(\mathbf{b}\hat{b})) / \#_{\mathbf{x}}^{\mathcal{B}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{b})) \\ &= \#_x^{\mathcal{B}}(\text{tp}_{\mathbf{b}}(x) = \text{tp}_{\mathbf{b}}(\hat{b})). \end{aligned} \quad (5)$$

Similarly, for r -tuples \mathbf{a} and \mathbf{b} such that $\text{tp}(\mathbf{a}) = \text{tp}(\mathbf{b})$, where $r \leq k-2$ (!), and for any a and b , there are \hat{a} and \hat{b} such that $\text{tp}(\mathbf{b}\hat{b}) = \text{tp}(\mathbf{a}\hat{a})$ and

$$\#_{xy}^{\mathcal{A}}(\text{tp}_{\mathbf{a}}(xy) = \text{tp}_{\mathbf{a}}(a\hat{a})) = \#_{xy}^{\mathcal{B}}(\text{tp}_{\mathbf{b}}(xy) = \text{tp}_{\mathbf{b}}(\hat{b}\hat{b})). \quad (6)$$

For the desired solution put

$$\begin{aligned} X_\emptyset &:= 1, \\ X_p &:= \delta(\text{tp}(\mathbf{a}), \text{tp}(\mathbf{b})) / \#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})), \\ &\quad \text{for } p = \mathbf{ab}, 0 < |p| < k. \end{aligned} \quad (7)$$

For the denominator note that $\#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})) = \#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{b}))$ whenever $\text{tp}(\mathbf{a}) = \text{tp}(\mathbf{b})$. Clearly $X_p \geq 0$. Note that $X_p \neq 0$ implies $\text{tp}(\mathbf{a}) = \text{tp}(\mathbf{b})$, which implies that $\text{atp}(\mathbf{a}) = \text{atp}(\mathbf{b})$ whereby $\mathbf{a} \mapsto \mathbf{b}$ is a local isomorphism.

We check that the given assignment to the variables X_p satisfies all instances of the equations $\text{CONT}(\ell)$ and $\text{COMP}(\ell)$ in Sherali–Adams of level $k-1$.

In fact, the X_p as specified by (7), satisfy all instances of the continuity equations $\text{CONT}(\ell)$ of levels $\ell \leq k$ (!) and all instances of the compatibility equations $\text{COMP}(\ell)$ of levels $\ell < k$, while level $k - 1$ Sherali–Adams just requires both equation types for levels $\ell < k$.

Consider an instance of $\text{CONT}(\ell)$ of level $\ell \leq k$, i.e., for $|p| < k$, with $p = \mathbf{ab}$, $a \in [n]$. If $\text{tp}(\mathbf{a}) \neq \text{tp}(\mathbf{b})$, then both sides of the equation are zero. In case $\text{tp}(\mathbf{a}) = \text{tp}(\mathbf{b})$, let $\hat{b} \in [n]$ be such that $\text{tp}(\mathbf{b}\hat{b}) = \text{tp}(\mathbf{aa})$ (such \hat{b} exist as $\text{tp}(\mathbf{a}) = \text{tp}(\mathbf{b})$ and since $|p| < k$). Then

$$\begin{aligned} \sum_{b'} X_{p \wedge ab'} &= \sum_{b'} \delta(\text{tp}(\mathbf{aa}), \text{tp}(\mathbf{bb}')) / \#_{\mathbf{xx}}(\text{tp}(\mathbf{xx}) = \text{tp}(\mathbf{aa})) \\ &= \#_x(\text{tp}_{\mathbf{b}}(x) = \text{tp}_{\mathbf{a}}(a)) / \#_{\mathbf{xx}}(\text{tp}(\mathbf{xx}) = \text{tp}(\mathbf{aa})) \\ &= \#_x(\text{tp}_{\mathbf{b}}(x) = \text{tp}_{\mathbf{b}}(\hat{b})) / \#_{\mathbf{xx}}(\text{tp}(\mathbf{xx}) = \text{tp}(\mathbf{b}\hat{b})) \\ &= \#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{b}))^{-1} = X_p, \end{aligned}$$

where the crucial equality leading to the last line is from equation (3).

Consider now an instance of equation $\text{COMP}(\ell)$ of level $\ell < k$, i.e., with $|p| < k - 1$, with $p = \mathbf{ab}$, $a \in [n]$, $b \in [n]$. Again, the case of $\text{tp}(\mathbf{a}) \neq \text{tp}(\mathbf{b})$ is trivial. So we are left with the case of $p = \mathbf{ab}$ with $\text{tp}(\mathbf{a}) = \text{tp}(\mathbf{b})$ and $|p| \leq k - 2$. These imply that there are \hat{a} and \hat{b} such that $\text{tp}(\mathbf{aa}\hat{a}) = \text{tp}(\mathbf{bb}\hat{b})$. Then

$$\begin{aligned} &\sum_{a'} A_{aa'} X_{p \wedge a'b} \\ &= \sum_{a'} A_{aa'} \delta(\text{tp}(\mathbf{aa}'), \text{tp}(\mathbf{bb})) / \#_{\mathbf{xx}}(\text{tp}(\mathbf{xx}) = \text{tp}(\mathbf{bb})) \\ &= \frac{\#_y(\text{edge}(ay) \wedge \text{tp}_{\mathbf{a}}(y) = \text{tp}_{\mathbf{a}}(\hat{a}))}{\#_{\mathbf{xx}}(\text{tp}(\mathbf{xx}) = \text{tp}(\mathbf{bb}))} \\ &= \frac{\#_{xy}(\text{edge}(xy) \wedge \text{tp}_{\mathbf{a}}(x) = \text{tp}_{\mathbf{a}}(a) \wedge \text{tp}_{\mathbf{a}}(y) = \text{tp}_{\mathbf{a}}(\hat{a}))}{\#_{\mathbf{xx}}(\text{tp}(\mathbf{xx}) = \text{tp}(\mathbf{bb})) \cdot \#_x(\text{tp}_{\mathbf{a}}(x) = \text{tp}_{\mathbf{a}}(a))} \\ &= \frac{\#_{xy}(\text{edge}(xy) \wedge \text{tp}_{\mathbf{a}}(x) = \text{tp}_{\mathbf{a}}(a) \wedge \text{tp}_{\mathbf{a}}(y) = \text{tp}_{\mathbf{a}}(\hat{a}))}{\#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{b})) \cdot \#_x(\text{tp}_{\mathbf{b}}(x) = \text{tp}_{\mathbf{b}}(b)) \cdot \#_x(\text{tp}_{\mathbf{a}}(x) = \text{tp}_{\mathbf{a}}(a))}, \end{aligned} \tag{8}$$

where we use instances of equation (3), and, in the passage from the third to the fourth line, artificially count over all realisations of $\text{tp}_{\mathbf{a}}(a)$ instead of just the fixed parameter a , and compensate for that in the denominator.

The counting term in the numerator of this expression,

$$\#_{xy}(\text{edge}(xy) \wedge \text{tp}_{\mathbf{a}}(x) = \text{tp}_{\mathbf{a}}(a) \wedge \text{tp}_{\mathbf{a}}(y) = \text{tp}_{\mathbf{a}}(\hat{a})),$$

is the sum of the number of realisations of all those types $(\text{tp}_{\mathbf{a}}(a''), \text{tp}_{\mathbf{a}}(a'))$ that simultaneously extend $\text{tp}_{\mathbf{a}}(a)$, $\text{tp}_{\mathbf{a}}(\hat{a})$ and contain the formula $\text{edge}(xy)$. Each one of these types has exactly the same number of realisations in \mathcal{A} as the corresponding type that simultaneously extends $\text{tp}_{\mathbf{b}}(\hat{b})$, $\text{tp}_{\mathbf{b}}(b)$ and contains the formula $\text{edge}(xy)$. By symmetry of the graphs under consideration, $\text{edge}(xy)$ is equivalent with $\text{edge}(yx)$ and what we obtained in (8) coincides with the corresponding evaluation of the right-hand side of this instance of equation $\text{COMP}(\ell)$ as desired:

$$\begin{aligned}
& \sum_{b'} B_{b'b} X_{p \hat{\wedge} ab'} \\
&= \sum_{b'} B_{b'b} \delta(\text{tp}(\mathbf{a}a), \text{tp}(\mathbf{b}b')) / \#_{\mathbf{x}x}(\text{tp}(\mathbf{x}x) = \text{tp}(\mathbf{a}a)) \\
&= \frac{\#_{xy}(\text{edge}(yx) \wedge \text{tp}_{\mathbf{b}}(x) = \text{tp}_{\mathbf{b}}(b) \wedge \text{tp}_{\mathbf{a}}(y) = \text{tp}_{\mathbf{a}}(a))}{\#_{\mathbf{x}x}(\text{tp}(\mathbf{x}x) = \text{tp}(\mathbf{a}a)) \cdot \#_x(\text{tp}_{\mathbf{b}}(x) = \text{tp}_{\mathbf{b}}(b))} \tag{9} \\
&= \frac{\#_{xy}(\text{edge}(yx) \wedge \text{tp}_{\mathbf{b}}(x) = \text{tp}_{\mathbf{b}}(b) \wedge \text{tp}_{\mathbf{b}}(y) = \text{tp}_{\mathbf{b}}(\hat{b}))}{\#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})) \cdot \#_x(\text{tp}_{\mathbf{a}}(x) = \text{tp}_{\mathbf{a}}(a)) \cdot \#_x(\text{tp}_{\mathbf{b}}(x) = \text{tp}_{\mathbf{b}}(b))} .
\end{aligned}$$

Corollary 5.1. *If $\mathcal{A} \equiv_{\mathcal{C}}^k \mathcal{B}$, then there is a solution (X_p) for the combination of the continuity equations $\text{CONT}(\ell)$ of levels $\ell \leq k$ (!) with the compatibility equations $\text{CONT}(\ell)$ of levels $\ell < k$.*

5.1.2 From a level $k - 1$ solution to $\mathbf{C}^{<k}$ -equivalence

In the following we discuss what it means that some admissible real or rational non-negative assignment to the variables X_p for all $|p| < k$ satisfies the equations $\text{CONT}(\ell)$ and $\text{COMP}(\ell)$ for $\ell < k$, i.e., $\text{ISO}(k-1)$.

Lemma 5.2. *If $(X_p)_{|p| < k}$ is a solution to $\text{ISO}(k-1)$, then $X_p \neq 0$ implies that*

- (a) *p is a local bijection; and, strengthening this, that*
- (b) *p is a local isomorphism.*

Proof. For (a) we only need to use instances of the continuity equations $\text{CONT}(\ell)$. Suppose that $p = \mathbf{a}\mathbf{b}$ is not a local bijection, w.l.o.g. (by symmetry) assume that there are a and $b_1 \neq b_2$ such that $(a, b_1), (a, b_2) \in p$. For $p_0 := p \setminus (a, b_2)$ we clearly have $\ell := |p_0| < k - 1$, and looking at the instance of $\text{CONT}(\ell)$ for this p_0 and a , we find that the two summands for $b' = b_i$, $i = 1, 2$, both contribute to the left-hand side. So the equation and non-negativity of all X -assignments imply that $X_{p_0} + X_p \leq X_{p_0}$, whence $X_p = 0$.

For (b) we use (a) and instances of the equations $\text{COMP}(\ell)$. The claim is true for $p = \emptyset$, and we lift it to all other p by induction. Note that for $|p| = 1$, $p = ab$ cannot fail to be a local isomorphism (in undirected, loop-free graphs).

Assume then that $X_{p \hat{\wedge} ab} > 0$, that $0 < |p| < k - 1$ and that (b) holds true for p . Note that equations $\text{CONT}(|p| + 1)$ and $X_{p \hat{\wedge} ab} > 0$ imply that $X_p > 0$. Hence, by the inductive hypothesis, p is a local isomorphism.

By (a), $p \hat{\wedge} ab$ is a local bijection, and we check that it also must be a local isomorphism. For this it remains to show that, for instance (a, a_1) is an edge of \mathcal{A} iff (b, b_1) is an edge of \mathcal{B} . Since the edge relations are symmetric, it suffices to show that

- (i) $A_{a_1, a} = 1 \Rightarrow B_{b_1, b} \neq 0$, and
- (ii) $B_{b, b_1} = 1 \Rightarrow A_{aa_1} \neq 0$.

For (i) we use this instance of equation $\text{COMP}(\ell)$ for $\ell := |p| + 1$:

$$\sum_{a'} A_{a_1 a'} X_{p \hat{\wedge} a' b} = \sum_{b'} X_{p \hat{\wedge} a_1 b'} B_{b' b}.$$

The right-hand side reduces to the single term $X_p B_{b_1 b}$ because $a_1 \in \text{dom}(p)$. As the left-hand side is positive if $A_{a_1, a} = 1$ and $X_{p \hat{\wedge} ab} > 0$, (i) follows.

An analogous argument for (ii) is based on the instance $\sum_{a'} A_{aa'} X_{p \hat{\wedge} a' b_1} = \sum_{b'} X_{p \hat{\wedge} ab'} B_{b' b_1}$ of equation $\text{COMP}(\ell)$. \square

$\mathbf{C}^{<k}$ -equivalence

A solution for the variables X_p satisfying $\text{ISO}(k-1)$ is in fact not strong enough to guarantee \mathbf{C}^k -equivalence, but a slightly lesser equivalence,

$$\mathcal{A} \equiv_{\mathbf{C}}^{<k} \mathcal{B},$$

which we characterise in terms of a modified, *weak bijective k -pebble game* over \mathcal{A}, \mathcal{B} . The game is played by two players. If $m \neq n$, player **II** loses immediately. Otherwise, a play of the game proceeds in a sequence of rounds. Positions of the game are sets $p \subseteq [m] \times [n]$ of size $|p| \leq k-1$. Normally, the initial position is \emptyset , but we will also consider plays of the game starting from other initial positions. A single round of the game, starting in position p , is played as follows.

1. If $|p| = k-1$, player **I** selects a pair $ab \in p$. If $|p| < k-1$, he omits this step.
2. Player **II** selects a bijection between $[m]$ and $[n]$ (recall that $m = n$).
3. Player **I** chooses a pair $a'b'$ from this bijection.
4. If $p^+ := p \hat{\wedge} a'b'$ is a local isomorphism then the new position is

$$p' := \begin{cases} (p \setminus ab) \hat{\wedge} a'b' & \text{if } |p| = k-1, \\ p \hat{\wedge} a'b' & \text{if } |p| < k-1. \end{cases}$$

Otherwise, the play ends and player **II** loses.

Player **II** wins a play if it lasts forever, i.e., if $m = n$ and she never loses in step 4 of a round.

Note that the weak bijective k -pebble game requires more of the second player than the bijective $(k-1)$ -pebble game, because p^+ rather than just p' is required to be a local isomorphism. On the other hand, it requires less than the bijective k -pebble game: the bijective k -pebble game precisely requires the second player to choose the bijection without prior knowledge of the pair ab that will be removed from the position. A strategy for player **II** in the weak version is good for the usual version if it is fully symmetric or uniform w.r.t. the pebble pair that is going to be removed.

However, this is only relevant if $k \geq 3$. The weak bijective 2-pebble game and the bijective 2-pebble game are essentially the same.

Definition 5.3. \mathcal{A} and \mathcal{B} are $\mathbf{C}^{<k}$ -equivalent, $\mathcal{A} \equiv_{\mathbf{C}}^{<k} \mathcal{B}$, if the second player has a winning strategy in the weak bijective k -pebble game on \mathcal{A}, \mathcal{B} .

Furthermore, for tuples \mathbf{a} and \mathbf{b} of the same length $\ell < k$ we let $\mathcal{A}, \mathbf{a} \equiv_{\mathbf{C}}^{<k} \mathcal{B}, \mathbf{b}$ if the second player has a winning strategy in the weak bijective k -pebble game on \mathcal{A}, \mathcal{B} with initial position \mathbf{ab} .

Observation 5.4. $\mathcal{A} \equiv_{\mathcal{C}}^2 \mathcal{B} \Leftrightarrow \mathcal{A} \equiv_{\mathcal{C}}^{\leq 2} \mathcal{B}$, and for all $k \geq 3$:

$$\mathcal{A} \equiv_{\mathcal{C}}^k \mathcal{B} \Rightarrow \mathcal{A} \equiv_{\mathcal{C}}^{\leq k} \mathcal{B} \Rightarrow \mathcal{A} \equiv_{\mathcal{C}}^{k-1} \mathcal{B}.$$

Remark 5.5. *The weak bijective k -pebble game is equivalent to a bisimulation-like game with $k - 1$ pebbles where in each round the first player may slide a pebble along an edge of one of the graphs and the duplicator has to answer by sliding the corresponding pebble along an edge of the other graph. In this version, the game corresponds to the $(k - 1)$ -pebble sliding game introduced by Atserias and Maneva [1]. They prove that equivalence of two graphs with respect to the $(k - 1)$ -pebble sliding game implies that $\text{ISO}(k - 1)$ has a solution. In view of the equivalence of the sliding game with our weak bijective k -pebble game, this implies the backward direction of Theorem 5.7 below.*

Let I_n be the set of positions of the weak bijective k -pebble game over \mathcal{A}, \mathcal{B} in which the second player has a strategy to survive through n rounds. Let \sim^n stand for the equivalence relation induced by I_n , i.e., the transitive closure of the relation that puts $\mathbf{a} \sim^n \mathbf{b}$ if $p = \mathbf{ab} \in I_n$. Note that \sim^n is compatible with permutations in the sense that, for instance, $\mathbf{a} \sim \mathbf{b}$ iff $\pi(\mathbf{a}) \sim \pi(\mathbf{b})$ for any $\pi \in S_n$. We write $\pi(\mathbf{a})$ for the application of the permutation $\pi \in S_n$ to the components of $\mathbf{a} = (a_1, \dots, a_n)$, which results in $\pi(\mathbf{a}) = (a_{\pi(1)}, \dots, a_{\pi(n)})$.

For $n = 0$, I_0 consists of all size $k - 1$ local isomorphisms. We characterise I_{n+1} and \sim^{n+1} in terms of I_n by means of back&forth conditions for a single round: $\mathbf{a} \sim^{n+1} \mathbf{b}$ ($p = \mathbf{ab} \in I_{n+1}$) iff position \mathbf{ab} is good in the following sense: for $1 \leq j \leq k - 1$, the second player has a response that guarantees a target position in I_n if the first player chooses index j .

I.e., for each $1 \leq j \leq k - 1$, the second player needs to have a between $[m]$ and $[n]$ such that for every $(a, b) \in \rho_j$

$$\text{atp}(\mathbf{aa}) = \text{atp}(\mathbf{bb}) \quad \text{and} \quad \mathbf{a}_j^a \mathbf{b}_j^b \in I_n.$$

The first condition says that $p \hat{=} ab$ is a local isomorphism, the second that the new position is good for n further rounds.

Note that, since \mathcal{A} is a graph, the quantifier-free type $\text{atp}(\mathbf{aa})$ is fully determined by $\text{atp}(\mathbf{a})$ and the $\text{atp}(a_i a)$ for $1 \leq i \leq k - 1$, which in turn are determined by $\text{atp}(\mathbf{a}_j^a a)$. The condition that $\text{atp}(\mathbf{a}) = \text{atp}(\mathbf{b})$ is a pre-condition for the round to be played; the condition that $\text{atp}(a_i a) = \text{atp}(b_i b)$ is part of the post-condition that $p \setminus (j) \hat{=} ab$ is a local isomorphism, for all i apart from $i = j$.

Let $(\alpha_i)_{i \in I}$ be an enumeration of the \sim^n -classes over \mathcal{A} and \mathcal{B} . Then the above conditions on membership of $p = \mathbf{ab}$ in I_{n+1} are equivalent to the following:

$$\begin{aligned} & \text{for each } 1 \leq j \leq k - 1, \\ & \text{for every } \sim^n\text{-class } \alpha, \text{ and} \\ & \text{for every quantifier-free type } \eta(x, y): \\ & \#_a^{\mathcal{A}}(\mathbf{a}_j^a \in \alpha \wedge \text{atp}(a_j a) = \eta) = \#_b^{\mathcal{B}}(\mathbf{b}_j^b \in \alpha \wedge \text{atp}(b_j b) = \eta). \end{aligned}$$

Note, towards the claimed equivalence, that these numerical equalities allow the second player to piece together a bijection that respects the partition of $[m]$

and $[n]$ according to different combinations of α and η , which in turn guarantees that any pair (a, b) drawn from the bijection respects this partition and hence leads to a position $\mathbf{a}_j^a \mathbf{b}_j^b \in I_n$ as required.

Conversely, if one of these equalities were violated, then any bijection will have to have at least one pair that does not respect the partition of $[m]$ and $[n]$ w.r.t. the α and η . If the first player picks such a bad pair (a, b) , then the second player loses during this round because $\text{atp}(\mathbf{a}\mathbf{a}) \neq \text{atp}(\mathbf{b}\mathbf{b})$, or the resulting new position $\mathbf{a}_j^a \mathbf{b}_j^b$ is not in I_n .

For later use we state the condition on full $\mathbf{C}^{<k}$ -equivalence, corresponding to the stable limit of the above refinement step. For $\mathbf{a} \in [m]^{k-1}$ and $\mathbf{b} \in [n]^{k-1}$, $\mathcal{A}, \mathbf{a} \equiv_{\mathbf{C}}^{<k} \mathcal{B}, \mathbf{b}$ iff

$$\begin{aligned} & \text{for each } 1 \leq j \leq k-1, \\ & \text{for all } \mathbf{C}^{<k}\text{-equivalence classes } \alpha, \text{ and} \\ & \text{for every quantifier-free type } \eta(x, y): \\ & \#_a^{\mathcal{A}}(\mathbf{a}_j^a \in \alpha \wedge \text{atp}(a_j a) = \eta) = \#_b^{\mathcal{B}}(\mathbf{b}_j^b \in \alpha \wedge \text{atp}(b_j b) = \eta). \end{aligned} \tag{10}$$

From local isomorphisms to $\mathbf{C}^{<k}$ -equivalence. We observe that for any solution (X_p) of the level $k-1$ equations, and for every $|p| \leq k-2$ such that $X_p \neq 0$, the matrix

$$\left(\frac{X_{p \wedge ab}}{X_p} \right)_{a \in [m], b \in [n]}$$

is doubly stochastic by equations $\text{CONT}(\ell)$. In particular, the continuity equations, even for $\ell = 0$, also enforce that \mathcal{A} and \mathcal{B} have the same number of vertices, and we may assume that $m = n$.

Lemma 5.6. *For $k \geq 3$, if $(X_{p \wedge ab})_{|p| \leq k-2, a \in [n], b \in [n]}$ is a solution to $\text{ISO}(k-1)$ then for all $\mathbf{a} \in [n]^{k-1}$ and $\mathbf{b} \in [n]^{k-1}$:*

$$X_{\mathbf{a}\mathbf{b}} > 0 \implies \mathcal{A}, \mathbf{a} \equiv_{\mathbf{C}}^{<k} \mathcal{B}, \mathbf{b}.$$

Proof. Consider tuples \mathbf{a} and \mathbf{b} of length $k-1$ such that $X_{\mathbf{a}\mathbf{b}} > 0$. It suffices to show that, for each $1 \leq j \leq k-1$, the second player has a response ρ_j in a single round played in component j that guarantees a resulting position $\mathbf{a}'\mathbf{b}' = \mathbf{a}_j^{a'} \mathbf{b}_j^{b'}$ for which again $X_{\mathbf{a}'\mathbf{b}'} > 0$.

Fix some j . Let $a := a_j$, $b := b_j$ and p such that $\mathbf{a}\mathbf{b} = p \wedge ab$.⁵ Since $X_{\mathbf{a}\mathbf{b}} > 0$, equations $\text{CONT}(\ell)$ imply that also $X_p > 0$. Note that $|p| \leq k-2$. The matrix Y defined by $Y_{ab} := X_{p \wedge ab}/X_p$ is doubly stochastic, with a strictly positive entry in the position ab under consideration.

By Corollary 3.16, $Z = YY^t$ and $Z' = Y^t Y$ are symmetric and doubly stochastic with positive entries on the diagonal and induce Y -related partitions $[n] = \bigcup_{i \in I} D_i$ and $[n] = \bigcup_{i \in I} D'_i$ that are stable w.r.t. A and B , respectively. As discussed in the proof of Theorem 4.3, cf. equation (2), the characteristic vectors \mathbf{d}_i and \mathbf{d}'_i of these stable partitions are related according to $\mathbf{d}'_i = Y^t \mathbf{d}_i$ and $\mathbf{d}_i =$

⁵Note that $\mathbf{a}\mathbf{b} = p \wedge ab$ just specifies the subset p consisting of pairs in $\mathbf{a} \mapsto \mathbf{b}$ other than (a, b) ; our notation should not wrongly suggest an appeal to ordered tuples.

$Y\mathbf{d}'_i$. Similarity of the partitions as stated in the proof of Theorem 4.3 implies that the partitions agree w.r.t. sizes of the partition sets, $|D_i| = |D'_i| = n_i$ and w.r.t. the characteristic counts $\nu_{ij}^A = \nu_{ij}^B$, where $\nu_{ij}^A = \mathbf{d}_i^t A \mathbf{d}_j$ and $\nu_{ij}^B = (\mathbf{d}'_i)^t B \mathbf{d}'_j$.

Because $X_{\mathbf{ab}} = X_{p \wedge ab} = Y_{ab} > 0$, $a \in D_k$ and $b \in D_k$ for the same $k \in I$. It follows that, for every $i \in I$,

$$|\{a' \in D_i : A_{aa'} = 1\}| = |\{b' \in D'_i : B_{bb'} = 1\}|.$$

For this observe that these counts are ν_{ki}/n_k . The second player may therefore choose a bijection that bijectively maps D_i to D'_i for $i \in I$ in such a manner that for every pair (a', b') in this bijection, (a, a') is an edge in \mathcal{A} iff (b, b') is an edge in \mathcal{B} .

If the first player now picks any pair (a', b') from this bijection, then $a' \in D_i$ and $b' \in D_i$ for some $i \in I$, and the Y -relatedness of the partitions implies that $Y_{a'b'} > 0$ and hence $Y_{a'b'} X_p = X_{p \wedge a'b'} > 0$. By Lemma 5.2 (b), $p \wedge a'b'$ is a local isomorphism; and so is, by assumption, $p \wedge ab$. As also (a, a') is an edge in \mathcal{A} iff (b, b') is an edge in \mathcal{B} by choice of the bijection, $p^+ := p \wedge ab \wedge a'b' = \mathbf{ab} \wedge a'b'$ is a local isomorphism, too. The second player is thus guaranteed to reach a resulting position $p' = \mathbf{a}'\mathbf{b}' = p \wedge a'b'$ for which $X_{p'} > 0$. \square

Theorem 5.7. *ISO($k - 1$) has a solution if, and only if, $\mathcal{A} \equiv_{\mathcal{C}}^{<k} \mathcal{B}$.*

Proof. The last lemma settles one implication. For the converse implication, it remains to argue that $\mathcal{C}^{<k}$ -equivalence suffices in place of \mathcal{C}^k -equivalence to provide a solution to the Sherali–Adams relaxation of level $k - 1$. We now let $\text{tp}(\mathbf{a})$ stand for the $\mathcal{C}^{<k}$ -type, or the $\mathcal{C}^{<k}$ -equivalence class of the tuple \mathbf{a} . We may look at just tuples of length $k - 1$, by trivial padding through repetition of the last component say. Put

$$\begin{aligned} X_{\emptyset} &:= 1 \\ X_p &:= \delta(\text{tp}(\mathbf{a}), \text{tp}(\mathbf{b})) / \#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})) \\ &\quad \text{for } p = \mathbf{ab}, 0 < |p| \leq k - 1. \end{aligned} \tag{11}$$

We know that $\mathcal{C}^{<k}$ -equivalence refines \mathcal{C}^{k-1} -equivalence, and that an assignment to X_p according to \mathcal{C}^{k-1} -types of $(k - 1)$ -tuples was shown above to satisfy the continuity equations $\text{CONT}(\ell)$ of levels $\ell < k$, cf. Corollary 5.1. One can infer from this that also the refinement used here satisfies these equations.

For satisfaction of equations $\text{COMP}(\ell)$ of level $\ell < k$, however, we need to appeal to something less than the extension property that boosts \mathbf{a} and \mathbf{b} to k -tuples $\mathbf{aa}\hat{a}$ and $\mathbf{bb}\hat{b}$ of the same \mathcal{C}^k -type, as we used in connection with (8) above.

Here as there, however, we only need to look at $p = \mathbf{ab}$ of size (up to) $k - 2$ for which $\mathcal{A}, \mathbf{a} \equiv_{\mathcal{C}}^{<k} \mathcal{B}, \mathbf{b}$, because all other instances of the equation are trivially true with 0 on both sides. We fix such p .

Now, for any combination of $\mathcal{C}^{<k}$ -types α and β of $(k - 1)$ -tuples and quantifier-free type η of a pair,

$$\begin{aligned} &\#_{aa'}^A(\text{tp}(\mathbf{aa}) = \alpha \wedge \text{tp}(\mathbf{aa}') = \beta \wedge \text{atp}(aa') = \eta) \\ &= \#_{bb'}^B(\text{tp}(\mathbf{bb}) = \alpha \wedge \text{tp}(\mathbf{bb}') = \beta \wedge \text{atp}(bb') = \eta). \end{aligned} \tag{12}$$

This follows from an analysis of the $C^{<k}$ -game from position $p = \mathbf{ab}$ through two rounds, in which the first player first gets the last pebble placed on any one of the possible choices for a , with responses b as provided by the second player's bijection (in exactly the same number); then the first player plays on that last component again, and replaces it with any one of the choices he may have for a' and its match b' according to the second player's bijection (again, the same number of positive choices).

For given a and b , let now $\alpha := \text{tp}(\mathbf{aa})$ and $\beta := \text{tp}(\mathbf{bb})$. Then

$$\begin{aligned}
& \sum_{a'} A_{aa'} X_{p \hat{\sim} a'b} \\
&= \sum_{a'} A_{aa'} \delta(\text{tp}(\mathbf{aa'}), \text{tp}(\mathbf{bb})) / \#_{\mathbf{x}x}(\text{tp}(\mathbf{x}x) = \text{tp}(\mathbf{bb})) \\
&= \frac{\#_{a'}^A(\text{tp}(\mathbf{aa'}) = \beta \wedge \text{edge}(aa'))}{\#_{\mathbf{x}a'}(\text{tp}(\mathbf{x}a') = \beta)} \\
&= \frac{\#_{aa'}^A(\text{tp}(\mathbf{aa}) = \alpha \wedge \text{tp}(\mathbf{aa'}) = \beta \wedge \text{edge}(aa'))}{\#_{\mathbf{x}a'}(\text{tp}(\mathbf{x}a') = \beta) \cdot \#_a(\text{tp}(\mathbf{aa}) = \alpha)} \\
&= \frac{\#_{aa'}^A(\text{tp}(\mathbf{aa}) = \alpha \wedge \text{tp}(\mathbf{aa'}) = \beta \wedge \text{edge}(aa'))}{\#_{a'}(\text{tp}(\mathbf{aa'}) = \beta) \cdot \#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})) \cdot \#_a(\text{tp}(\mathbf{aa}) = \alpha)}.
\end{aligned}$$

We transform this term further, using (12), a renaming of dummy variables in counting terms and the symmetry of the unique quantifier-free type η determined by $\text{edge}(xy)$ in simple undirected graphs. The goal is to show equality with the corresponding term obtained for $\sum_{b'} X_{p \hat{\sim} ab'} B_{b'b}$. Equality (12) is used in the first step of these transformations, starting from the term just obtained:

$$\begin{aligned}
& \frac{\#_{aa'}^A(\text{tp}(\mathbf{aa}) = \alpha \wedge \text{tp}(\mathbf{aa'}) = \beta \wedge \text{edge}(aa'))}{\#_{a'}(\text{tp}(\mathbf{aa'}) = \beta) \cdot \#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{a})) \cdot \#_a(\text{tp}(\mathbf{aa}) = \alpha)} \\
&= \frac{\#_{bb'}^B(\text{tp}(\mathbf{bb}) = \alpha \wedge \text{tp}(\mathbf{bb'}) = \beta \wedge \text{edge}(bb'))}{\#_{b'}(\text{tp}(\mathbf{bb'}) = \beta) \cdot \#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{b})) \cdot \#_b(\text{tp}(\mathbf{bb}) = \alpha)} \\
&= \frac{\#_{bb'}^B(\text{tp}(\mathbf{bb'}) = \alpha \wedge \text{tp}(\mathbf{bb}) = \beta \wedge \text{edge}(bb'))}{\#_b(\text{tp}(\mathbf{bb}) = \beta) \cdot \#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{b})) \cdot \#_{b'}(\text{tp}(\mathbf{bb'}) = \alpha)} \\
&= \frac{\#_{b'}^B(\text{tp}(\mathbf{bb'}) = \alpha \wedge \text{edge}(bb'))}{\#_{\mathbf{x}}(\text{tp}(\mathbf{x}) = \text{tp}(\mathbf{b})) \cdot \#_{b'}(\text{tp}(\mathbf{bb'}) = \alpha)} \\
&= \sum_{b'} B_{b'b} \delta(\text{tp}^{<k}(\mathbf{bb'}), \text{tp}^{<k}(\mathbf{aa})) / \#_{\mathbf{x}x}(\text{tp}(\mathbf{x}x) = \text{tp}^{<k}(\mathbf{aa})) \\
&= \sum_{b'} X_{p \hat{\sim} ab'} B_{b'b}.
\end{aligned}$$

□

5.2 The gap

Based on a construction due to Cai, Fürer, and Immerman [5], for $k \geq 3$ we construct graphs showing that $\mathcal{A} \equiv_C^{<k} \mathcal{B} \not\equiv_C^k \mathcal{A} \equiv_C^k \mathcal{B}$, and that $\mathcal{A} \equiv_C^{k-1} \mathcal{B} \not\equiv_C^k \mathcal{A} \equiv_C^k \mathcal{B}$.

$\mathcal{A} \equiv_{\mathbb{C}}^{< k} \mathcal{B}$. So the implications in Observation 5.4 are strict for $k \geq 3$.

Example 5.8. For every $k \geq 3$, there are graphs \mathcal{A} and \mathcal{B} such that $\mathcal{A} \equiv_{\mathbb{C}}^{k-1} \mathcal{B}$ but $\mathcal{A} \not\equiv_{\mathbb{C}}^{< k} \mathcal{B}$.

Proof. We present the argument explicitly for $k = 4$; its variant for $k = 3$ and the generalisation to higher k are straightforward. For \mathcal{A} and \mathcal{B} we use the straight and the twisted version of the Cai–Fürer–Immerman companions of the 4-clique.

We use copies of the standard degree 3 gadget

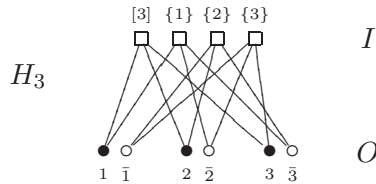
$$\begin{aligned} H_3 &:= (O \cup I, E), \text{ where} \\ O &:= \{1, 2, 3\} \cup \{\bar{1}, \bar{2}, \bar{3}\} \quad (\text{outer nodes}) \\ I &:= \mathcal{P}_{\text{odd}}(\{1, 2, 3\}) \quad (\text{inner nodes: odd subsets}) \\ E &:= \{\{i, s\} : i \in O, s \in I, i \in s\} \cup \{\{\bar{i}, s\} : i \in O, s \in I, i \notin s\} \end{aligned}$$

and its dual

$$\begin{aligned} \bar{H}_3 &:= (O \cup I, E), \text{ where} \\ O &:= \{1, 2, 3\} \cup \{\bar{1}, \bar{2}, \bar{3}\} \quad (\text{outer nodes}) \\ I &:= \mathcal{P}_{\text{even}}(\{1, 2, 3\}) \quad (\text{inner nodes: even subsets}) \\ E &:= \{\{i, s\} : i \in O, s \in I, i \in s\} \cup \{\{\bar{i}, s\} : i \in O, s \in I, i \notin s\}. \end{aligned}$$

In each of these, we think of the three pairs of outer nodes as positive markers $(1, 2, 3)$ and negative markers $(\bar{1}, \bar{2}, \bar{3})$ for the elements of the set $[3] = \{1, 2, 3\}$, and of the four inner nodes as subsets $s \subseteq [3]$ (of odd cardinalities in the case of H_3 , and of even cardinalities in the case of \bar{H}_3); the edges incident with a particular $s \in I$ encode elementhood of $i = 1, 2, 3$ in s by linking s to i if $i \in s$ and to \bar{i} if $i \notin s$. Both graphs are bipartite with inner nodes of degree 3 and outer nodes of degree 2, which serve as ports to link copies of H_3 and \bar{H}_3 . We really use coloured variants of H_3 and \bar{H}_3 that distinguish the vertices of the distinct copies of H_3 and \bar{H}_3 , and inner and outer as well as the three groups of port vertices (i.e., $\{i, \bar{i}\}$ for $i = 1, 2, 3$) within each of them. This is without loss of generality, since we may eliminate colours, e.g., by attaching simple, disjoint paths of different lengths to the members of each group of vertices.

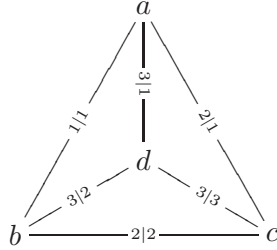
The non-trivial automorphisms of this decorated variant of H_3 and \bar{H}_3 precisely allow for simultaneous swaps within exactly two pairs of port vertices. In the sketch we distinguish positive element markers from negative ones by using filled and open circles; this is just to highlight the combinatorial source of the graph structure, and in (the decorated versions of) H_3 and \bar{H}_3 this distinction is *not* present.



Let \mathcal{A} consist of four decorated copies of H_3 , copies a, b, c, d say, that are linked by edges in corresponding outer nodes:

- $(a, 1)$ is linked to $(b, 1)$ and $(a, \bar{1})$ to $(b, \bar{1})$,
- $(a, 2)$ is linked to $(c, 1)$ and $(a, \bar{2})$ to $(c, \bar{1})$,
- $(a, 3)$ is linked to $(d, 1)$ and $(a, \bar{3})$ to $(d, \bar{1})$,
- $(b, 2)$ is linked to $(c, 2)$ and $(b, \bar{2})$ to $(c, \bar{2})$,
- $(d, 2)$ is linked to $(b, 3)$ and $(d, \bar{2})$ to $(b, \bar{3})$,
- $(d, 3)$ is linked to $(c, 3)$ and $(d, \bar{3})$ to $(c, \bar{3})$.

In short: bridges are built between the 1-ports of $b/c/d$ with the 1/2/3-ports of a ; between the 2-ports of b and c ; and between the 2/3-ports of d and the 3-ports of b/c .



\mathcal{B} consists of three decorated copies of H_3 (labelled a, b, c) and one of \bar{H}_3 (labelled d), and linked in the same manner.

We speak of the vertex sets in the individual decorated copies of H_3 and \bar{H}_3 in \mathcal{A} and \mathcal{B} as *regions* a, b, c and d .

- Observation 5.9.** (a) *The automorphism groups of both \mathcal{A} and \mathcal{B} are such that only the trivial automorphism fixes any three inner vertices from three distinct regions. Fixing one inner vertex each in two different regions leaves precisely one non-trivial automorphism, which swaps the two bridges between the outer vertices connecting the remaining two regions.*
- (b) *Any three corresponding regions in \mathcal{A} and \mathcal{B} are linked by a local isomorphism. Any local isomorphism between two corresponding regions of \mathcal{A} and \mathcal{B} has precisely two extensions to each one of the remaining two regions, which are related by a swap of the bridges between those two regions.*

Extensions of these assertions to structures similarly obtained from k -cliques for $k > 4$ are straightforward.

Property (b) can be used to show that $\mathcal{A} \equiv_{\mathcal{C}}^3 \mathcal{B}$, by exhibiting a strategy for the second player that maintains a local isomorphism between the unions of the pebbled regions.

We now argue that $\mathcal{A} \not\equiv_{\mathcal{C}}^{<4} \mathcal{B}$. The first player can initially force a position in which pebble i in \mathcal{A} is on the (positive) port node (a, i) for $i = 1, 2, 3$; w.l.o.g. (viz., up to an automorphism of \mathcal{B}) the pebbles in \mathcal{B} are on (a, i) as well.

Next we let the first player move pebbles 1 and 2 along paths of length 2 to the ports in copies b and c : pebble 1 to $(b, 1)$, pebble 2 to $(c, 1)$. Necessarily, over \mathcal{B} , these pebbles will then also be on the nodes with these labels.

In the next two steps, we let the first player move these two pebbles along edges to the inner nodes $(b, [3])$ and $(c, [3])$ in copies b and c . The forced responses in \mathcal{B} will put pebble 1 to one of $(b, \{1\})$ or $(b, [3])$, and pebble 2

to one of $(c, \{1\})$ or $(c, [3])$. The two skew combinations $((b, \{1\}), (c, [3]))$ or $((b, [3]), (c, \{1\}))$ for pebbles 1 and 2 are bad for the second player, because the two pebbles end up at distance greater than 3 in \mathcal{B} while their distance in \mathcal{A} is 3 – the first player can force a win in two rounds involving pebble 3. Up to an automorphism of \mathcal{B} that fixes the location of the third pebble, we may therefore assume that the pebble configuration is $((b, [3]), (c, [3]), (a, 3))$ in both \mathcal{A} and \mathcal{B} .

In further moves along edges that take all three pebbles towards the port nodes of the d -regions in both \mathcal{A} and \mathcal{B} , the first player forces the configuration $((d, 2), (d, 3), (d, 1))$ in both \mathcal{A} and \mathcal{B} .

Since the d -region of \mathcal{A} is a copy of H_3 while that of \mathcal{B} is a copy of \bar{H}_3 , however, all three pebbles have edges to the inner node $(d, [3])$ in \mathcal{A} , but there is no such node in \mathcal{B} . So a single C^k -round in which the fourth pebble in \mathcal{A} is put on $(d, [3])$, lets the first player win the game (the first player can also win by moving one of the 3 pebbles along an edge in \mathcal{A} to $(d, [3])$). \square

Example 5.10. For every $k \geq 3$, there are graphs \mathcal{A} and \mathcal{B} such that $\mathcal{A} \equiv_C^k \mathcal{B}$ but $\mathcal{A} \not\equiv_C^k \mathcal{B}$.

Proof. We describe the argument for the case $k = 3$, where we use variants of \mathcal{A} and \mathcal{B} as in the last proof, but with one marked inner node: in both \mathcal{A} and \mathcal{B} we mark the inner node $(a, [3])$ by a new colour (which can be eliminated by attaching a path of some characteristic length, as observed above). We denote these modified structures as \mathcal{A}_* and \mathcal{B}_* . In effect this means that the second player needs to respect moves to these marked vertices as if they were coloured in both the C^3 - and the $C^{<3}$ -game: if the second player fails to pair $(a, [3])^{\mathcal{A}_*}$ with $(a, [3])^{\mathcal{B}_*}$, this mismatched pair would allow the first player an easy win.

We claim that $\mathcal{A}_* \not\equiv_C^3 \mathcal{B}_*$ while $\mathcal{A}_* \equiv_C^3 \mathcal{B}_*$.

First, for $\mathcal{A}_* \not\equiv_C^3 \mathcal{B}_*$, we let the first player play the first three rounds so that the inner nodes $(b, [3])$, $(c, [3])$ and $(d, [3])$ are pebbled in \mathcal{A}_* , and (unless the second player has lost already or will lose for trivial reasons involving the decorations) matched with inner nodes (b, s_b) , (c, s_c) and some (d, s_d) in \mathcal{B}_* , which means that $s_b, s_c \subseteq [3]$ are of odd size while $s_d \subseteq [3]$ is of even size. It follows that between at least two pairs of nodes from $((a, [3]), (b, [3]), (c, [3]), (d, [3]))^{\mathcal{A}_*}$ and $((a, [3]), (b, s_b), (c, s_c), (d, s_d))^{\mathcal{B}_*}$, distances in \mathcal{A}_* and \mathcal{B}_* are different: the nodes in \mathcal{A}_* are at pairwise distance 3; for at least one pair of the nodes in \mathcal{B}_* the distance is greater than 3. This is easily turned into a strategy for the first player to pebble along one of these short connecting paths in \mathcal{A}_* , alternating between two pebbles; this forces a mismatch w.r.t. to the target node, which is either pebbled (if in regions b, c, d) or coloured with the special marker path (if in region a), and in either situation the second player can be made to lose.

For $\mathcal{A}_* \equiv_C^3 \mathcal{B}_*$ we claim that the second player can maintain the condition that the current configuration $(a_1, a_2; b_1, b_2) \in \text{dom}(\mathcal{A}_*)^2 \times \text{dom}(\mathcal{B}_*)^2$ extends to a local isomorphism on the union of the a -region with those regions to which a_1 and a_2 (and thus b_1 and b_2) belong. In fact we may add an extra virtual pebble pair on $a_0 := (a, [3])^{\mathcal{A}_*}$ and $b_0 := (a, [3])^{\mathcal{B}_*}$ and maintain a local isomorphism ξ whose domain consists of up to three out of the four regions and such that $\xi(a_i) = b_i$ for $i = 0, 1, 2$. Suppose, w.l.o.g., that in such a situation the first

player announces play on pebble 2, i.e., that the pair (a_2, b_2) will be withdrawn at the end of the round. Let ξ_0 be the restriction of ξ to the a -region and the region of a_1/b_1 . Since ξ_0 covers at most two of the four regions, Observation 5.9 guarantees extensions to local isomorphisms that

- (a) cover any one of the remaining (two or three) regions, and
- (b) at the same time respect a given pairing between the outer nodes of that new region in the direction of one of the (one or two) further remaining regions.

From such extensions, the second player can piece together a bijection that allows her to maintain the desired condition, as follows. The chosen bijection extends ξ to the (one or two) regions not covered by ξ as follows.

Case 1: a_2/b_2 are inner nodes or outer nodes in the direction of a region covered by ξ_0 . Extend ξ by bijections obtained from extensions of ξ_0 to local isomorphisms involving one extra region at a time, as in (a).

Case 2: a_2/b_2 are outer nodes in the direction of a further region not covered by ξ_0 . Extend ξ to that further region according to an extension of ξ_0 as a local isomorphism that also respects the neighbours of a_2/b_2 in this region, in the sense of (b); the extension to a remaining region (if there is such) can be completed as in Case 1.

Any bijection pieced together like this is a good choice:

- the second player does not lose during this round: any pair selected from the bijection belongs to a local isomorphism extending ξ_0 and thus comprising a_0/b_0 and a_1/b_1 and respects a_2/b_2 as well as $N(a_2)/N(b_2)$;
- the second player maintains the local isomorphism condition: the extension of ξ_0 by that part of the bijection that covers the region of the new pair may serve as the new ξ' .

It follows that the second player has a strategy to respond indefinitely, so that $\mathcal{A}_* \equiv_{\mathcal{C}}^{\leq 3} \mathcal{B}_*$. \square

Corollary 5.11. *The level of equivalence captured by the Sherali–Adams relaxation of fractional graph isomorphism of level $k - 1$ is strictly between \mathcal{C}^{k-1} -equivalence and \mathcal{C}^k -equivalence, for every $k \geq 3$.*

5.3 Closing the gap

As before, we let \mathcal{A}, \mathcal{B} be graphs with vertex sets $[m], [n]$, respectively, and we let A, B be their adjacency matrices. We use variables X_p for set $p \subseteq [m] \times [n]$ of size $|p| \leq k$. For each $1 \leq j \leq k$ let $J \in \{0, 1\}^{[n]^k \times [n]^k}$ be the adjacency matrix of the j -th accessibility relation, which relates two k -tuples if they coincided in all but their j th component. We would like to put the extra condition that $JX = XJ$, where we think of the family $(X_p)_{|p|=k}$ as one square matrix with rows and columns indexed by $[m]^k$ and $[n]^k$, respectively. For a particular choice

of j , this condition $JX = XJ$ translates into

$$\sum_a X_{\mathbf{a}_j^a \mathbf{b}} = \sum_b X_{\mathbf{a} \mathbf{b}_j^b},$$

for all $\mathbf{a} \in [m]^k$, $\mathbf{b} \in [n]^k$, $a \in [m]$ and $b \in [n]$. For this we just observe that J has entries 1 precisely for all tuples $\mathbf{a}\mathbf{a}'$ and $\mathbf{b}\mathbf{b}'$ where $\mathbf{a}' = \mathbf{a}_j^a$ or $\mathbf{b}' = \mathbf{b}_j^b$ for some $a \in [m]$ or $b \in [n]$. Note also that J is fully invariant under the action of permutations (of $[m]$ or $[n]$) on the k -tuples indexing its rows and columns.

If we look at the indices p as *sets* of pairs over $[m] \times [n]$ again, we want to impose the additional requirement of permutation-invariance on the original X , which we had thought of as in terms of variables $X_{\mathbf{a}\mathbf{b}}$ indexed by tuples of pairs over $[m] \times [n]$. Let us adopt momentarily the notation $p \setminus (j)$ for the result of removing the j -th pair (a_j, b_j) from $p = \mathbf{a}\mathbf{b}$. Then, up to the obvious permutation of the resulting tuple, $p' = \mathbf{a}_j^a \mathbf{b}_j^b = \mathbf{a}\mathbf{b} \setminus (j) \hat{\ } ab$. Under the natural assumption of permutation invariance, the above can now be re-written into

$$\sum_a X_{p \setminus (j) \hat{\ } ab} = \sum_b X_{p \setminus (j) \hat{\ } ab},$$

for $|p| = k$, $a \in [m]$, $b \in [n]$, $1 \leq j \leq k$, and hence to the familiar format

$$\sum_a X_{p \hat{\ } ab} = \sum_b X_{p \hat{\ } ab},$$

for $|p| = k - 1$, $a \in [m]$, $b \in [n]$, which is a consequence of Sherali–Adams equations $\text{CONT}(\ell)$ of level $\ell = k$ (one up!).

Note that, as is always the case for the continuity equations, these conditions make no reference to the edge relations of \mathcal{A} and \mathcal{B} .

We now combine the equations $\text{COMP}(\ell)$, concerning compatibility with the edge relations, of level $\ell < k$ with the continuity equations $\text{CONT}(\ell)$ of levels $\ell \leq k$.

| | |
|---|--|
| $\text{ISO}(k - 1/2)$ | |
| $\left. \begin{array}{l} X_\emptyset = 1 \quad \text{and} \\ X_p = \sum_{b'} X_{p \hat{\ } ab'} = \sum_{a'} X_{p \hat{\ } a'b} \\ \text{for } p < k, a \in [n], b \in [m] \end{array} \right\}$ | $\text{CONT}(\ell) \text{ for } \ell \leq k$ |
| $\left. \begin{array}{l} \sum_{a'} A_{aa'} X_{p \hat{\ } a'b} = \sum_{b'} X_{p \hat{\ } ab'} B_{b'b} \\ \text{for } p < k - 1, a \in [n], b \in [m] \end{array} \right\}$ | $\text{COMP}(\ell) \text{ for } \ell < k$ |
| $X_p \geq 0 \text{ for } p \leq k$ | |

We know from Corollary 5.1 that \mathbf{C}^k -equivalence of simple graphs implies the existence of a solution for exactly this combination of equations. We now want to show that conversely, a solution to $\text{ISO}(k - 1/2)$ yields a strategy for the second player in the bijective k -pebble game, i.e., implies \mathbf{C}^k -equivalence.

First some preparation concerning the solution space of the equations.

Lemma 5.12. *Let $(X_p)_{|p| \leq k}$ be a solution and $\ell \geq 1$ a natural number. Then $(\hat{X}_p)_{|p| \leq k}$ is also a solution where \hat{X}_p is defined by induction on $|p|$ according to*

$$\begin{aligned}\hat{X}_\emptyset &:= X_\emptyset = 1 \\ \hat{X}_{p \wedge ab} &:= X_{p \wedge ab} = 0 && \text{if } X_p = 0, \\ \hat{X}_{p \wedge ab} &:= \hat{X}_p((YY^t)^\ell Y)_{ab} && \text{if } X_p > 0 \text{ and } Y_{ab} := 1/X_p X_{p \wedge ab}.\end{aligned}$$

Proof. W.l.o.g. $[m] = [n] = [n]$. The continuity equations involving the matrix $X = (X_{p \wedge ab})_{a,b \in [n]}$ are preserved under multiplication from the left by arbitrary doubly stochastic matrices of the form $Z = (Z_{aa'})_{a,a' \in [n]}$ (just as under multiplication from the right by some doubly stochastic $Z' = (Z_{bb'})$). We note that $Z = YY^t = XX^t/X_p^2$ is doubly stochastic by the given continuity equations for $X = (X_{p \wedge ab})_{a,b \in [n]}$. It follows that $\hat{X} = (\hat{X}_{p \wedge ab})_{a,b \in [n]}$ satisfies the new continuity equations which stipulate row- and column-sums \hat{X}_p for this matrix.

For consistency with the view of the \hat{X}_p as being indexed by *sets* of pairs, we need to verify that $\hat{X}_{p \wedge ab} = \hat{X}_p$ whenever $ab \in p$. But in that case, already $X_{p \wedge ab} = X_p$ was the only non-zero entry in the row of a as well as in the column of b , by the given continuity equations. It follows that $(YY^t)_{aa'} = 1/X_p^2 \sum_{b'} X_{p \wedge ab'} X_{p \wedge a'b'} = (1/X_p) X_{p \wedge a'b} = \delta(a', a)$ so that also $\hat{X}_{p \wedge ab} = \hat{X}_p/X_p X_{p \wedge ab} = \hat{X}_p$ as desired.

Compatibility equations of the form $AX = XB$ are compatible with multiplication of X by $Z = XX^t$ from the left, whenever A and B are symmetric. We note that the adjacency matrices A and B commute with $Z = XX^t$ and $Z' = X^t X$ by the given compatibility equations.

Passage from $X = X_{p \wedge ab}$ and X_p to $\hat{X}_{p \wedge ab}$ and \hat{X}_p therefore preserves all equations of level $k - 1/2$. \square

For the following recall the definition of a *good* matrix without null rows or columns from Definition 3.5.

Definition 5.13. Call a solution $(X_p)_{|p| \leq k}$ a *good solution* if, whenever $X_p > 0$ for $|p| < k$, the associated doubly stochastic matrix $Y = (1/X_p)(X_{p \wedge ab})_{a,b \in [n]}$ is good in the sense of Definition 3.5.

Corollary 5.14. *If there is any solution $(X_p)_{|p| \leq k}$, then there is a good solution. For a good solution $(X_p)_{|p| \leq k}$ and $|p| < k$ with $X_p \neq 0$, let Y be the doubly stochastic matrix $Y := (X_{p \wedge ab})_{a,b \in [n]}$. Then the symmetric matrices $Z = YY^t$ and $Z' = Y^t Y$ are good symmetric and induce Y/Y^t -related partitions $[n] = \bigcup_i D_i$ and $[n] = \bigcup_i D'_i$, and satisfy*

- (i) $Y_{D_i D'_i} > 0$ for all i , and
- (ii) $Y_{D_i D'_j} = 0$ for all $i \neq j$.

Proof. An application of Lemma 5.12 with $\ell \geq n - 1$ produces a good solution from any given solution. The stated property for doubly stochastic matrices Y induced by a good solution follows directly from Corollary 3.9. \square

Lemma 5.15. *If $(X_p)_{|p| \leq k}$ is a good solution to $\text{ISO}(k - 1/2)$, then for all $\mathbf{a} \in [n]^k$ and $\mathbf{b} \in [n]^k$:*

$$X_{\mathbf{ab}} > 0 \implies \mathcal{A}, \mathbf{a} \equiv_{\mathcal{C}}^k \mathcal{B}, \mathbf{b}.$$

Proof. For $k = 2$, we know that even the level 1 equations suffice. We therefore assume that $k \geq 3$ and fix a good solution $(X_p)_{|p| \leq k}$. From the proof of Lemma 5.2 (a) we know that $X_p > 0$ implies that $p = \mathbf{ab}$ is a local bijection, while (b) from Lemma 5.2 tells us that at least every $p = \mathbf{ab}$ of size up to $k - 1$ with $X_p > 0$ must be a local isomorphism. But for $k \geq 3$ and simple graphs the local isomorphism property for all p of size $k - 1$ with $X_p > 0$ implies the same for $p = \mathbf{ab}$ of size k , essentially by monotonicity as imposed by the continuity equations:

Let $p = \mathbf{ab}$, $|p| = k$, $X_p > 0$. Then the continuity equations imply that $X_q > 0$ for every restriction $q \subseteq p$. E.g., if $p = q \hat{\wedge} ab$, then $X_q = \sum_{a'} X_{q \hat{\wedge} a'b} \geq X_{q \hat{\wedge} ab} = X_p$ shows that $X_q > 0$. But if every size $k - 1$ restriction of p is a local isomorphism, then so is p itself. Here it is important that $k \geq 3$ is strictly larger than the arity of the relations in \mathcal{A} and \mathcal{B} , the edge relation in this case.

It remains to argue that the second player has a strategy to maintain the condition that $X_p > 0$ in the bijective k -pebble game on positions $p = \mathbf{ab}$. I.e., for a single round played from a position $p \hat{\wedge} ab$, where $p = \mathbf{ab}$ is of size up to $k - 1$:

if $X_{p \hat{\wedge} ab} > 0$, then there is a bijection ρ between $[m]$ and $[n]$
such that for every pair $(a', b') \in \rho$, also $X_{p \hat{\wedge} a'b'} > 0$.

Fix p of size up to $k - 1$ with $X_p > 0$, and let Y be the doubly stochastic matrix with entries $Y_{ab} := (1/X_p)X_{p \hat{\wedge} ab}$. Let $Z := YY^t$ and $Z' := Y^tY$ be the induced symmetric doubly stochastic matrices with positive entries on the diagonal as considered in Lemma 3.8. Let $[n] = \bigcup_{i \in I} D_i$ and $[n] = \bigcup_{i \in I} D'_i$ be the Y -related partitions of $[n] = [m]$ induced by Z and Z' , respectively. Then $|D_i| = |D'_i|$ for all $i \in I$ by Lemma 3.7. So there is a bijection that is compatible with these two partitions in the sense that it associates D_i bijectively to D'_i . Any choice of a pair (a', b') from such a bijection corresponds to an entry $X_{p \hat{\wedge} a'b'}$ with $a' \in D_i$ and $b' \in D'_i$ for the same $i \in I$; because (X_p) is a good solution, this means that the corresponding entry $Y_{a'b'}$ is positive, i.e., that $X_{p \hat{\wedge} a'b'} > 0$, as desired. So, if the second player chooses such a bijection, the resulting position p' is guaranteed to have positive $X_{p'}$ again. \square

The following theorem sums up the results of the previous lemmas and should be compared to Theorem 5.7 for $\text{ISO}(k - 1)$.

Theorem 5.16. *$\text{ISO}(k - 1/2)$ has a solution if, and only if, $\mathcal{A} \equiv_{\mathcal{C}}^k \mathcal{B}$.*

5.4 Boolean arithmetic and \mathbf{L}^k -equivalence

We saw in Section 4.2 that equations, which are direct consequences of the basic continuity and compatibility equations w.r.t. the adjacency matrices A

and B , may carry independent weight in their boolean interpretation. This is no surprise, because the boolean reading is much weaker, especially due to the absorptive nature of \vee , which unlike $+$ does not allow for inversion. $AX = XB$ for doubly stochastic X and $A, B \in \mathbb{B}^{n,n}$ implies $A^c X = X B^c$. Similarly, we found in part (a) of Lemma 5.2 that the continuity equations imply that p is a local bijection whenever $X_p > 0$, under real arithmetic; this also fails for boolean arithmetic.

We now augment the boolean requirements by corresponding boolean equations that express

- (a) compatibility also w.r.t. A^c and B^c , as in boolean fractional isomorphism,
- (b) the new constraint $X_p = 0$ whenever p is not a local bijection.

In the presence of the continuity equations, which force monotonicity, it suffices for (b) to force $X_{aa'bb'} = 0$ for all $a, a' \in [m]$, $b, b' \in [n]$ such that *not* $a = a' \Leftrightarrow b = b'$. This is captured by the constraint MATCH(2) below. Together with the continuity and compatibility equations, MATCH(2) then implies that $X_p = 0$ unless p is a local isomorphism, just as in the proof of part (b) of Lemma 5.2, also in terms of boolean arithmetic.

So we now use the following boolean version of the Sherali–Adams hierarchy $\text{ISO}(k-1)$ and $\text{ISO}(k-1/2)$ for $k \geq 2$.

| | |
|--|--|
| <p>B-ISO($k-1$)</p> <div style="display: flex; justify-content: space-between; align-items: center; margin-top: 10px;"> <div style="flex: 1;"> $\left. \begin{aligned} X_\emptyset &= 1 \quad \text{and} \\ X_p &= \sum_{b'} X_{p \wedge ab'} = \sum_{a'} X_{p \wedge a'b} \\ \text{for } p < k, a \in [m], b \in [n] \end{aligned} \right\}$ </div> <div style="flex: 0.5; text-align: center;"> $\text{CONT}(\ell) \text{ for } \ell < k$ </div> </div> <div style="display: flex; justify-content: space-between; align-items: center; margin-top: 10px;"> <div style="flex: 1;"> $\left. \begin{aligned} X_{ab \wedge ab'} &= 0 = X_{ab \wedge a'b} \\ \text{for } a \neq a' \in [m], b \neq b' \in [n] \end{aligned} \right\}$ </div> <div style="flex: 0.5; text-align: center;"> $\text{MATCH}(2)$ </div> </div> <div style="display: flex; justify-content: space-between; align-items: center; margin-top: 10px;"> <div style="flex: 1;"> $\left. \begin{aligned} \sum_{a'} A_{aa'} X_{p \wedge a'b} &= \sum_{b'} X_{p \wedge ab'} B_{b'b} \\ \text{for } p < k-1, a \in [m], b \in [n] \end{aligned} \right\}$ </div> <div style="flex: 0.5; text-align: center;"> $\text{COMP}(\ell) \text{ for } \ell < k$ </div> </div> <div style="display: flex; justify-content: space-between; align-items: center; margin-top: 10px;"> <div style="flex: 1;"> $\left. \begin{aligned} \sum_{a'} A_{aa'}^c X_{p \wedge a'b} &= \sum_{b'} X_{p \wedge ab'} B_{b'b}^c \\ \text{for } p < k-1, a \in [m], b \in [n] \end{aligned} \right\}$ </div> <div style="flex: 0.5; text-align: center;"> $\text{COMP}(\ell)^c \text{ for } \ell < k$ </div> </div> | |
|--|--|

For B-ISO($k-1/2$) we just require $\text{CONT}(\ell)$ for all $\ell \leq k$, i.e., additionally for $\ell = k$.

Remark 5.17. B-ISO($k-1$) and B-ISO($k-1/2$) are systems of boolean equations, and the reader may wonder whether they can be solved efficiently. At first sight, it may seem NP-complete to solve such systems (just like boolean satisfiability). However, our systems consist of “linear” equations of the following

forms:

$$\sum_{i \in I} X_i = \sum_{j \in J} X_j, \quad (13)$$

$$\sum_{i \in I} X_i = 0, \quad (14)$$

$$\sum_{i \in I} X_i = 1. \quad (15)$$

(The equations of the form (14) are actually subsumed by those of the form (13) with $J = \emptyset$.) It is an easy exercise to prove that such systems of linear boolean equations can be solved in polynomial time.

The *weak* k -pebble game is the straightforward adaptation of the weak bijective k -pebble game to the setting without counting. A single round of the game is played as follows.

1. If $|p| = k - 1$, player **I** selects a pair $ab \in p$. If $|p| < k - 1$, he omits this step.
2. Player **I** chooses an element a' of \mathcal{A} or b' of \mathcal{B} .
3. Player **II** answers with an element b' of \mathcal{B} or a' of \mathcal{A} , respectively.
4. If $p^+ := p \hat{\ } a'b'$ is a local isomorphism then the new position is

$$p' := \begin{cases} (p \setminus ab) \hat{\ } a'b' & \text{if } |p| = k - 1, \\ p \hat{\ } a'b' & \text{if } |p| < k - 1. \end{cases}$$

Otherwise, the play ends and player **II** loses.

We denote weak k -pebble equivalence as in $\mathcal{A} \equiv_{\perp}^{<k} \mathcal{B}$ and extend this to $\mathcal{A}, \mathbf{a} \equiv_{\perp}^{<k} \mathcal{B}, \mathbf{b}$ for tuples \mathbf{a}, \mathbf{b} of the same length $< k$. We sketch a proof of the following, which is a boolean analogue of the correspondences between half-step levels of Sherali–Adams and \mathbf{C}^k - and $\mathbf{C}^{<k}$ -equivalence established in the last section.

Theorem 5.18. (a) B-ISO($k - 1$) has a solution (w.r.t. boolean arithmetic) if, and only if, $\mathcal{A} \equiv_{\perp}^{<k} \mathcal{B}$.
 (b) B-ISO($k - 1/2$) has a solution (w.r.t. boolean arithmetic) if, and only if, $\mathcal{A} \equiv_{\perp}^k \mathcal{B}$.

Proof. We start with the second part of the theorem. For the backward direction, suppose that $\mathcal{A} \equiv_{\perp}^k \mathcal{B}$ and let, for $p = \mathbf{ab}$ of size $|p| \leq k$,

$$X_p := \begin{cases} 1 & \text{if } \mathcal{A}, \mathbf{a} \equiv_{\perp}^k \mathcal{B}, \mathbf{b}, \\ 0 & \text{else.} \end{cases}$$

Clearly this assignment satisfies MATCH(2), and one easily checks that it also satisfies the boolean continuity equations CONT(ℓ) for $\ell \leq k$. For the boolean

compatibility equations $\text{COMP}(\ell)$ and $\text{COMP}(\ell)^c$ for $\ell < k$, let us check, for instance, an equation $\text{COMP}(k-1)$. The non-trivial case is that of $p = \mathbf{ab}$ where $\mathbf{a} \in [n]^{k-2}$ and $\mathbf{b} \in [m]^{k-2}$ are such that $\mathcal{A}, \mathbf{a} \equiv_{\mathcal{L}}^k \mathcal{B}, \mathbf{b}$ so that $X_p = 1$. Consider the instance of equation $\text{CONT}(k-1)$ for $a \in [m], b \in [n]$:

$$\sum_{a'} A_{aa'} X_{p \wedge a'b} = \sum_{b'} X_{p \wedge ab'} B_{b'b}.$$

Since $\mathcal{A}, \mathbf{a} \equiv_{\mathcal{L}}^k \mathcal{B}, \mathbf{b}$, there is a $\hat{b} \in [m]$ such that $\mathcal{A}, \mathbf{a} \equiv_{\mathcal{L}}^k \mathcal{B}, \mathbf{b}\hat{b}$. Suppose the left-hand side of the equation evaluates to 1. This means that there is an edge in \mathcal{A} from a to some a' for which $X_{p \wedge a'b} = 1$, i.e., for which $\mathcal{A}, \mathbf{a}a' \equiv_{\mathcal{L}}^k \mathcal{B}, \mathbf{b}b$.

In other words, there is an edge in \mathcal{A} from some a' for which $\mathcal{A}, \mathbf{a}a' \equiv_{\mathcal{L}}^k \mathcal{B}, \mathbf{b}b$ to some a for which $\mathcal{A}, \mathbf{a}a \equiv \mathcal{B}, \mathbf{b}\hat{b}$. So every realisation of the \mathcal{L}^k -type of $\mathcal{B}, \mathbf{b}b$ has an edge between b and some b' where $\mathcal{B}, \mathbf{b}b' \equiv_{\mathcal{L}}^k \mathcal{A}, \mathbf{a}a$, which implies that the right-hand side of the equation evaluates to 1, too.

For the forward direction, we extract from a good solution to $\text{ISO}(k-1/2)$ a strategy for the second player to maintain pebbles in configurations \mathbf{ab} for which $X_{\mathbf{ab}} = 1$. Let $p = \mathbf{ab}$ of size $|p| < k$ be such that the current position is $p \wedge ab$, where $X_{p \wedge ab} = 1$, and let the first player move the pebble from a to a' in \mathcal{A} , say. The second player needs to find some b' in \mathcal{B} such that again $X_{p \wedge a'b'} = 1$.

Analogous to the real case, a *good solution* is one where all the matrices $Y_{ab} = X_{p \wedge ab}$ for $X_p \neq 0$ (which are necessarily without null rows or columns), are such that the Y -related partitions of $[n]$ and $[m]$ induced by $Z = YY^t$ and $Z' = Y^tY$ put a and b in related partition sets if, and only if, $Y_{ab} = 1$. Here again, it suffices to postulate that Z and Z' are good symmetric, and an arbitrary solution can be turned into a good solution on the basis of Lemma 3.10.

So, if the second player picks any $b' \in [m]$ for which $Y_{a'b'} = 1$, this makes sure that $X_{p \wedge a'b'} = 1$ is maintained, and that $p \wedge a'b'$ is a local isomorphism.

We turn to part (a) of the theorem.

For the forward direction, we want to extract from a good (!) solution a strategy for the player **II** in the weak k -pebble game that maintains positions p s.t. $X_p = 1$. Recall that positions are now of size $< k$. Consider a position $p = \mathbf{aabb}$ of size $|p| = k-1$ with $X_p = 1$. Suppose that player **I** selects ab in the first step of the next round (“he announces to withdraw the pebble pair on ab ”) and selects a' in the second step (“he places a pebble on a' ”). W.l.o.g. suppose that $a' \neq a$, because $a' = a$ has the obvious response $b' := b$. Player **II** needs to find some $b' \in [m]$ such that $p^+ = p \wedge a'b'$ is a local isomorphism and for $p' = (p \setminus ab) \wedge ab$ also $X_{p'} = 1$. It suffices to make sure that $X_{p'} = 1$, that $b' \neq b$, and that bb' is an edge in \mathcal{B} iff aa' is an edge in \mathcal{A} . Suppose, for instance, that aa' is not an edge, i.e., that $A_{aa'} = 0$.

Let $p^- = p \setminus ab$, and let Y be the matrix with entries $Y_{a''b''} = X_{p^- \wedge a''b''}$. Let $[m] = \dot{\bigcup}_i D_i$ and $[n] = \dot{\bigcup}_i D'_i$ the partitions induced by YY^t and Y^tY , which are boolean bi-stable for A and B , respectively, and Y -related. Suppose $a \in D_i$ and $a' \in D_j$, so that $A_{aa'} = 0$ implies that $\iota_{ij}^{A^c} = 1$. Since $Y_{ab} = 1$, we have $b \in D'_i$; and as $\iota_{ij}^{B^c} = \iota_{ij}^{A^c} = 1$, there is also some $b' \in D'_j$ for which $B_{bb'}^c = 1$,

so that bb' is not an edge in \mathcal{B} and $b' \neq b$. As we are dealing with a good solution, $a' \in D_j$ and $b' \in D'_j$ imply that $Y_{a'b'} = 1$, so that $X_{p'} = X_{p' \wedge a'b'} = 1$.

For the backward direction, suppose that $\mathcal{A} \equiv_{<k} \mathcal{B}$ and let $X_\emptyset := 1$ and, for $\mathbf{a} \in [n]^{k-1}$ and $\mathbf{b} \in [m]^{k-1}$, $X_{\mathbf{ab}} := 1$ iff $\mathcal{A}, \mathbf{a} \equiv_{\leq k} \mathcal{B}, \mathbf{b}$. It is clear that this assignment satisfies $\text{MATCH}(2)$ and $\text{CONT}(\ell)$ for $\ell < k$. Consider then an instance of $\text{COMP}(\ell)$ for $\ell < k$,

$$\sum_{a'} A_{aa'} X_{p \wedge a'b} = \sum_{b'} X_{p \wedge ab'} B_{b'b}, \quad (16)$$

where $a \in [n], b \in [m], |p| < k-1, p = \mathbf{ab}$. Let us assume that $|p| = k-2$; this is the most difficult case. If $X_p = 0$ then $X_{p \wedge a'b'} = 0$ for all $a'b'$, and thus equation (16) is trivially satisfied. So assume $X_p = 1$, that is, $\mathcal{A}, \mathbf{a} \equiv_{\leq k} \mathcal{B}, \mathbf{b}$. Suppose for instance that the left-hand side of equation (16) evaluates to 1, i.e., that there is some a' adjacent to a in \mathcal{A} for which $\mathcal{A}, \mathbf{aa'} \equiv_{\leq k} \mathcal{B}, \mathbf{bb}$. Consider the weak k -pebble game in position $\mathbf{aa'bb}$. Assume player **I** selects the pair $a'b$ in the first step of the next round and selects a in the second step. Let b' be the answer of **II** when she plays according to her winning strategy. Then $\mathbf{aa'a} \mapsto \mathbf{bbb'}$ is a local isomorphism and the new position $\mathbf{aabb'}$ is a winning position for player **II**, that is, $\mathcal{A}, \mathbf{aa} \equiv_{\leq k} \mathcal{B}, \mathbf{bb'}$. Since $\mathbf{aa'a} \mapsto \mathbf{bbb'}$ is a local isomorphism and aa' is an edge of \mathcal{A} , the pair bb' is an edge of \mathcal{B} and thus $B_{b'b} = 1$. Since $\mathcal{A}, \mathbf{aa} \equiv_{\leq k} \mathcal{B}, \mathbf{bb'}$, we have $X_{p \wedge ab'} = 1$. Thus the right-hand side of equation (16) evaluates to 1 as well. \square

Remark 5.19. For all $k \geq 3$, $\equiv_{\leq k}^{k-1}, \equiv_{\leq k}^{<k}, \equiv_{\leq k}^k$ form a strictly increasing hierarchy of discriminating power.

Proof. The examples for the gaps between $\equiv_{\leq k}^{k-1}, \equiv_{\leq k}^{<k}, \equiv_{\leq k}^k$ given in Section 5.2, are in fact good in the setting without counting. The strategy analysis given there does not involve counting in any non-trivial manner. \square

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